```
cast_top.txt
Remarks ../../tmp/hicup_btcpxq_23790/CHO_top.txt
Remarks Created by XPLO2D V. 000310/2.8.7 at Fri May 26 17:27:19 2000 for
root
Remarks Auto-generated by XPLO2D from file ../../tmp/hicup_btcpxq_
23790/user.pdb
Remarks You *MUST* check/edit MASSes and CHARges !!!
Remarks Check DONOrs and ACCEptors
Remarks Verify IMPROpers yourself
Remarks DIHEdrals which are not flat are commented out

 set echo=false end

 { edit masses if necessary }
 MASS CX1    12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX2     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX3     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX4    12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX5     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX6    12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX7     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX8    12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX9     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX10    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX11   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX12    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX13   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS CX14   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX15    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX16    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX17   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX18    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX19   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX20    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX21   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS CX22   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX23    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX24    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX25   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX26    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX27    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX28   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS CX29   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX30    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX31   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX32    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX33    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX34   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX35    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX36    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX37   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX38    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX39   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX40    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX41    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX42    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX43   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX44    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX45    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX46    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX47   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
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 MASS HX48    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX49   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX50    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX51    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX52    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX53   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX54    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX55   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX56    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX57   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX58    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX59   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX60    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX61   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX62    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX63    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX64    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX65   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX66    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX67    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX68    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX69   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX70    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX71    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX72    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS OX73   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
 MASS HX74    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS OX75   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
 MASS HX76    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS OX77   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
 MASS OX78   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
 MASS HX79    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS OX80   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
 MASS HX81    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)

 autogenerate angles=true end

RESIdue CHO

GROUp
 ATOM  C1   TYPE CX1   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H11  TYPE HX2   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H12  TYPE HX3   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C2   TYPE CX4   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H2   TYPE HX5   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C3   TYPE CX6   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H3   TYPE HX7   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C4   TYPE CX8   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H41  TYPE HX9   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H42  TYPE HX10  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C5   TYPE CX11  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H5   TYPE HX12  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C6   TYPE CX13  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C7   TYPE CX14  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H71  TYPE HX15  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H72  TYPE HX16  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C8   TYPE CX17  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H8   TYPE HX18  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C9   TYPE CX19  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H9   TYPE HX20  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C10  TYPE CX21  CHARge  0.0  END ! Nr of Hs =  0
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ATOM  C11  TYPE CX22  CHARge  0.0  END ! Nr of Hs =  0
ATOM H111  TYPE HX23  CHARge  0.0  END ! Nr of Hs =  0
ATOM H112  TYPE HX24  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C12  TYPE CX25  CHARge  0.0  END ! Nr of Hs =  0
ATOM H121  TYPE HX26  CHARge  0.0  END ! Nr of Hs =  0
ATOM H122  TYPE HX27  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C13  TYPE CX28  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C14  TYPE CX29  CHARge  0.0  END ! Nr of Hs =  0
ATOM  H14  TYPE HX30  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C15  TYPE CX31  CHARge  0.0  END ! Nr of Hs =  0
ATOM H151  TYPE HX32  CHARge  0.0  END ! Nr of Hs =  0
ATOM H152  TYPE HX33  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C16  TYPE CX34  CHARge  0.0  END ! Nr of Hs =  0
ATOM H161  TYPE HX35  CHARge  0.0  END ! Nr of Hs =  0
ATOM H162  TYPE HX36  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C17  TYPE CX37  CHARge  0.0  END ! Nr of Hs =  0
ATOM  H17  TYPE HX38  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C18  TYPE CX39  CHARge  0.0  END ! Nr of Hs =  0
ATOM H181  TYPE HX40  CHARge  0.0  END ! Nr of Hs =  0
ATOM H182  TYPE HX41  CHARge  0.0  END ! Nr of Hs =  0
ATOM H183  TYPE HX42  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C19  TYPE CX43  CHARge  0.0  END ! Nr of Hs =  0
ATOM H191  TYPE HX44  CHARge  0.0  END ! Nr of Hs =  0
ATOM H192  TYPE HX45  CHARge  0.0  END ! Nr of Hs =  0
ATOM H193  TYPE HX46  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C20  TYPE CX47  CHARge  0.0  END ! Nr of Hs =  0
ATOM  H20  TYPE HX48  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C21  TYPE CX49  CHARge  0.0  END ! Nr of Hs =  0
ATOM H211  TYPE HX50  CHARge  0.0  END ! Nr of Hs =  0
ATOM H212  TYPE HX51  CHARge  0.0  END ! Nr of Hs =  0
ATOM H213  TYPE HX52  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C22  TYPE CX53  CHARge  0.0  END ! Nr of Hs =  0
ATOM  H22  TYPE HX54  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C23  TYPE CX55  CHARge  0.0  END ! Nr of Hs =  0
ATOM  H23  TYPE HX56  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C24  TYPE CX57  CHARge  0.0  END ! Nr of Hs =  0
ATOM  H24  TYPE HX58  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C25  TYPE CX59  CHARge  0.0  END ! Nr of Hs =  0
ATOM  H25  TYPE HX60  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C26  TYPE CX61  CHARge  0.0  END ! Nr of Hs =  0
ATOM H261  TYPE HX62  CHARge  0.0  END ! Nr of Hs =  0
ATOM H262  TYPE HX63  CHARge  0.0  END ! Nr of Hs =  0
ATOM H263  TYPE HX64  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C27  TYPE CX65  CHARge  0.0  END ! Nr of Hs =  0
ATOM H271  TYPE HX66  CHARge  0.0  END ! Nr of Hs =  0
ATOM H272  TYPE HX67  CHARge  0.0  END ! Nr of Hs =  0
ATOM H273  TYPE HX68  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C28  TYPE CX69  CHARge  0.0  END ! Nr of Hs =  0
ATOM H281  TYPE HX70  CHARge  0.0  END ! Nr of Hs =  0
ATOM H282  TYPE HX71  CHARge  0.0  END ! Nr of Hs =  0
ATOM H283  TYPE HX72  CHARge  0.0  END ! Nr of Hs =  0
ATOM  O1   TYPE OX73  CHARge  0.0  END ! Nr of Hs =  0
ATOM  HO1  TYPE HX74  CHARge  0.0  END ! Nr of Hs =  0
ATOM  O2   TYPE OX75  CHARge  0.0  END ! Nr of Hs =  0
ATOM  HO2  TYPE HX76  CHARge  0.0  END ! Nr of Hs =  0
ATOM  O3   TYPE OX77  CHARge  0.0  END ! Nr of Hs =  0
ATOM  O4   TYPE OX78  CHARge  0.0  END ! Nr of Hs =  0
ATOM  HO4  TYPE HX79  CHARge  0.0  END ! Nr of Hs =  0
ATOM  O5   TYPE OX80  CHARge  0.0  END ! Nr of Hs =  0
ATOM  HO5  TYPE HX81  CHARge  0.0  END ! Nr of Hs =  0
```

```
 BOND  C1   H11      BOND  C1   H12      BOND  C1   C2       BOND  C1   C10
 BOND  C2   H2       BOND  C2   C3       BOND  C2   O1       BOND  C3   H3
 BOND  C3   C4       BOND  C3   O2       BOND  C4   H41      BOND  C4   H42
 BOND  C4   C5       BOND  C5   H5       BOND  C5   C6       BOND  C5   C10
 BOND  C6   C7       BOND  C6   O3       BOND  C7   H71      BOND  C7   H72
 BOND  C7   C8       BOND  C8   H8       BOND  C8   C9       BOND  C8   C14
 BOND  C9   H9       BOND  C9   C10      BOND  C9   C11      BOND  C10  C19
 BOND  C11 H111      BOND  C11 H112      BOND  C11  C12      BOND  C12 H121
 BOND  C12 H122      BOND  C12  C13      BOND  C13  C14      BOND  C13  C17
 BOND  C13  C18      BOND  C14  H14      BOND  C14  C15      BOND  C15 H151
 BOND  C15 H152      BOND  C15  C16      BOND  C16 H161      BOND  C16 H162
 BOND  C16  C17      BOND  C17  H17      BOND  C17  C20      BOND  C18 H181
 BOND  C18 H182      BOND  C18 H183      BOND  C19 H191      BOND  C19 H192
 BOND  C19 H193      BOND  C20  H20      BOND  C20  C21      BOND  C20  C22
 BOND  C21 H211      BOND  C21 H212      BOND  C21 H213      BOND  C22  H22
 BOND  C22  C23      BOND  C22  O4       BOND  C23  H23      BOND  C23  O5
 BOND  C23  C24      BOND  C24  H24      BOND  C24  C25      BOND  C24  C28
 BOND  C25  H25      BOND  C25  C26      BOND  C25  C27      BOND  C26 H261
 BOND  C26 H262      BOND  C26 H263      BOND  C27 H271      BOND  C27 H272
 BOND  C27 H273      BOND  C28 H281      BOND  C28 H282      BOND  C28 H283
 BOND  O1   HO1      BOND  O2   HO2      BOND  O4   HO4      BOND  O5   HO5

 { edit these IMPRopers if necessary }
 IMPRoper  C1   H11  H12  C2  ! chirality or flatness improper    41.34
 IMPRoper  C1   C2   C3   H3  ! dihedral improper                179.06
 IMPRoper  C2   C1   O1   H2  ! chirality or flatness improper    33.65
 IMPRoper  C3   C2   O2   C4  ! chirality or flatness improper   -36.60
 IMPRoper  C4   C3   H41  H42 ! chirality or flatness improper    33.35
 IMPRoper  C5   C6   H5   C4  ! chirality or flatness improper   -36.70
 IMPRoper  C6   C5   O3   C7  ! chirality or flatness improper     0.00
 IMPRoper  C7   C6   H71  H72 ! chirality or flatness improper    35.02
 IMPRoper  C8   C7   H8   C9  ! chirality or flatness improper    38.11
 IMPRoper  C9   C8   H9   C10 ! chirality or flatness improper   -36.70
 IMPRoper  C10  C1   C5   C9  ! chirality or flatness improper   -36.06
 IMPRoper  C11  C9  H111 H112 ! chirality or flatness improper    32.90
 IMPRoper  C12  C11 H121 H122 ! chirality or flatness improper    33.25
 IMPRoper  C13  C12  C14  C17 ! chirality or flatness improper   -39.96
!IMPRoper  C13  C17  C20  H20 ! dihedral improper                  59.41
!IMPRoper  C13  C17  C20  C21 ! dihedral improper                 -60.57
 IMPRoper  C14  C8   C13  H14 ! chirality or flatness improper    29.90
 IMPRoper  C15  C14 H151 H152 ! chirality or flatness improper    33.01
 IMPRoper  C16  C15 H161 H162 ! chirality or flatness improper    33.71
 IMPRoper  C17  C13  C16  H17 ! chirality or flatness improper   -27.26
 IMPRoper  C18  C13 H181 H182 ! chirality or flatness improper   -33.15
 IMPRoper  C19  C10 H191 H192 ! chirality or flatness improper   -33.10
 IMPRoper  C20  C17  H20  C21 ! chirality or flatness improper    35.53
 IMPRoper  C21  C20 H211 H212 ! chirality or flatness improper   -33.45
 IMPRoper  C22  C20  O4   H22 ! chirality or flatness improper    33.69
 IMPRoper  C23  C22  H23  O5  ! chirality or flatness improper    33.59
 IMPRoper  C24  C23  C28  H24 ! chirality or flatness improper    33.81
 IMPRoper  C25  C24  H25  C26 ! chirality or flatness improper    35.22
 IMPRoper  C26  C25 H261 H262 ! chirality or flatness improper   -33.48
 IMPRoper  C27  C25 H271 H272 ! chirality or flatness improper   -33.43
 IMPRoper  C28  C24 H281 H282 ! chirality or flatness improper   -33.43

 { edit any DONOrs and ACCEptors if necessary }
 ACCEptor  O1   C2
 ACCEptor  O2   C3
 ACCEptor  O3   C6
 ACCEptor  O4   C22
 ACCEptor  O5   C23
```

```
END { RESIdue CHO }



cast_par.txt
Remarks ../../tmp/hicup_btcpxq_23790/CHO_par.txt
Remarks Created by XPLO2D V. 000310/2.8.7 at Fri May 26 17:27:19 2000 for
root
Remarks Auto-generated by XPLO2D from file ../../tmp/hicup_btcpxq_
23790/user.pdb
Remarks Parameters for residue type CHO

 set echo=false end

 { edit if necessary }
 BOND CX1  HX2    1000.0  1.090 ! Nobs =    1
 BOND CX1  HX3    1000.0  1.090 ! Nobs =    1
 BOND CX1  CX4    1000.0  1.461 ! Nobs =    1
 BOND CX1  CX21   1000.0  1.663 ! Nobs =    1
 BOND CX4  HX5    1000.0  1.090 ! Nobs =    1
 BOND CX4  CX6    1000.0  1.439 ! Nobs =    1
 BOND CX4  OX73   1000.0  1.393 ! Nobs =    1
 BOND CX6  HX7    1000.0  1.090 ! Nobs =    1
 BOND CX6  CX8    1000.0  1.559 ! Nobs =    1
 BOND CX6  OX75   1000.0  1.393 ! Nobs =    1
 BOND CX8  HX9    1000.0  1.089 ! Nobs =    1
 BOND CX8  HX10   1000.0  1.090 ! Nobs =    1
 BOND CX8  CX11   1000.0  1.437 ! Nobs =    1
 BOND CX11 HX12   1000.0  1.090 ! Nobs =    1
 BOND CX11 CX13   1000.0  1.594 ! Nobs =    1
 BOND CX11 CX21   1000.0  1.603 ! Nobs =    1
 BOND CX13 CX14   1000.0  1.483 ! Nobs =    1
 BOND CX13 OX77   1000.0  1.200 ! Nobs =    1
 BOND CX14 HX15   1000.0  1.090 ! Nobs =    1
 BOND CX14 HX16   1000.0  1.090 ! Nobs =    1
 BOND CX14 CX17   1000.0  1.533 ! Nobs =    1
 BOND CX17 HX18   1000.0  1.090 ! Nobs =    1
 BOND CX17 CX19   1000.0  1.594 ! Nobs =    1
 BOND CX17 CX29   1000.0  1.598 ! Nobs =    1
 BOND CX19 HX20   1000.0  1.090 ! Nobs =    1
 BOND CX19 CX21   1000.0  1.437 ! Nobs =    1
 BOND CX19 CX22   1000.0  1.603 ! Nobs =    1
 BOND CX21 CX43   1000.0  1.599 ! Nobs =    1
 BOND CX22 HX23   1000.0  1.090 ! Nobs =    1
 BOND CX22 HX24   1000.0  1.090 ! Nobs =    1
 BOND CX22 CX25   1000.0  1.577 ! Nobs =    1
 BOND CX25 HX26   1000.0  1.090 ! Nobs =    1
 BOND CX25 HX27   1000.0  1.090 ! Nobs =    1
 BOND CX25 CX28   1000.0  1.514 ! Nobs =    1
 BOND CX28 CX29   1000.0  1.526 ! Nobs =    1
 BOND CX28 CX37   1000.0  1.555 ! Nobs =    1
 BOND CX28 CX39   1000.0  1.576 ! Nobs =    1
 BOND CX29 HX30   1000.0  1.091 ! Nobs =    1
 BOND CX29 CX31   1000.0  1.521 ! Nobs =    1
 BOND CX31 HX32   1000.0  1.090 ! Nobs =    1
 BOND CX31 HX33   1000.0  1.090 ! Nobs =    1
 BOND CX31 CX34   1000.0  1.473 ! Nobs =    1
 BOND CX34 HX35   1000.0  1.090 ! Nobs =    1
 BOND CX34 HX36   1000.0  1.090 ! Nobs =    1
 BOND CX34 CX37   1000.0  1.528 ! Nobs =    1
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```
BOND CX37 HX38   1000.0  1.090 ! Nobs =    1
BOND CX37 CX47   1000.0  1.521 ! Nobs =    1
BOND CX39 HX40   1000.0  1.090 ! Nobs =    1
BOND CX39 HX41   1000.0  1.090 ! Nobs =    1
BOND CX39 HX42   1000.0  1.090 ! Nobs =    1
BOND CX43 HX44   1000.0  1.090 ! Nobs =    1
BOND CX43 HX45   1000.0  1.090 ! Nobs =    1
BOND CX43 HX46   1000.0  1.090 ! Nobs =    1
BOND CX47 HX48   1000.0  1.090 ! Nobs =    1
BOND CX47 CX49   1000.0  1.481 ! Nobs =    1
BOND CX47 CX53   1000.0  1.509 ! Nobs =    1
BOND CX49 HX50   1000.0  1.090 ! Nobs =    1
BOND CX49 HX51   1000.0  1.090 ! Nobs =    1
BOND CX49 HX52   1000.0  1.090 ! Nobs =    1
BOND CX53 HX54   1000.0  1.090 ! Nobs =    1
BOND CX53 CX55   1000.0  1.481 ! Nobs =    1
BOND CX53 OX78   1000.0  1.393 ! Nobs =    1
BOND CX55 HX56   1000.0  1.091 ! Nobs =    1
BOND CX55 CX57   1000.0  1.479 ! Nobs =    1
BOND CX55 OX80   1000.0  1.393 ! Nobs =    1
BOND CX57 HX58   1000.0  1.090 ! Nobs =    1
BOND CX57 CX59   1000.0  1.511 ! Nobs =    1
BOND CX57 CX69   1000.0  1.484 ! Nobs =    1
BOND CX59 HX60   1000.0  1.090 ! Nobs =    1
BOND CX59 CX61   1000.0  1.476 ! Nobs =    1
BOND CX59 CX65   1000.0  1.484 ! Nobs =    1
BOND CX61 HX62   1000.0  1.090 ! Nobs =    1
BOND CX61 HX63   1000.0  1.090 ! Nobs =    1
BOND CX61 HX64   1000.0  1.090 ! Nobs =    1
BOND CX65 HX66   1000.0  1.090 ! Nobs =    1
BOND CX65 HX67   1000.0  1.090 ! Nobs =    1
BOND CX65 HX68   1000.0  1.090 ! Nobs =    1
BOND CX69 HX70   1000.0  1.090 ! Nobs =    1
BOND CX69 HX71   1000.0  1.090 ! Nobs =    1
BOND CX69 HX72   1000.0  1.090 ! Nobs =    1
BOND OX73 HX74   1000.0  1.030 ! Nobs =    1
BOND OX75 HX76   1000.0  1.030 ! Nobs =    1
BOND OX78 HX79   1000.0  1.030 ! Nobs =    1
BOND OX80 HX81   1000.0  1.030 ! Nobs =    1

{ edit if necessary }
ANGLe HX2  CX1  HX3     500.0   111.22 ! Nobs =    1
ANGLe HX2  CX1  CX4     500.0   107.68 ! Nobs =    1
ANGLe HX2  CX1  CX21    500.0   106.75 ! Nobs =    1
ANGLe HX3  CX1  CX4     500.0   107.66 ! Nobs =    1
ANGLe HX3  CX1  CX21    500.0   106.75 ! Nobs =    1
ANGLe CX4  CX1  CX21    500.0   116.82 ! Nobs =    1
ANGLe CX1  CX4  HX5     500.0   108.22 ! Nobs =    1
ANGLe CX1  CX4  CX6     500.0   114.58 ! Nobs =    1
ANGLe CX1  CX4  OX73    500.0   108.22 ! Nobs =    1
ANGLe HX5  CX4  CX6     500.0   107.57 ! Nobs =    1
ANGLe HX5  CX4  OX73    500.0   110.69 ! Nobs =    1
ANGLe CX6  CX4  OX73    500.0   107.57 ! Nobs =    1
ANGLe CX4  CX6  HX7     500.0   111.78 ! Nobs =    1
ANGLe CX4  CX6  CX8     500.0   114.15 ! Nobs =    1
ANGLe CX4  CX6  OX75    500.0   108.33 ! Nobs =    1
ANGLe HX7  CX6  CX8     500.0   106.39 ! Nobs =    1
ANGLe HX7  CX6  OX75    500.0   108.24 ! Nobs =    1
ANGLe CX8  CX6  OX75    500.0   107.73 ! Nobs =    1
ANGLe CX6  CX8  HX9     500.0   107.96 ! Nobs =    1
ANGLe CX6  CX8  HX10    500.0   107.93 ! Nobs =    1
```

```
ANGLe CX6  CX8  CX11    500.0   109.48 ! Nobs =    1
ANGLe HX9  CX8  HX10    500.0   110.97 ! Nobs =    1
ANGLe HX9  CX8  CX11    500.0   104.36 ! Nobs =    1
ANGLe HX10 CX8  CX11    500.0   113.27 ! Nobs =    1
ANGLe CX8  CX11 HX12    500.0   107.91 ! Nobs =    1
ANGLe CX8  CX11 CX13    500.0   110.99 ! Nobs =    1
ANGLe CX8  CX11 CX21    500.0   119.85 ! Nobs =    1
ANGLe HX12 CX11 CX13    500.0   110.99 ! Nobs =    1
ANGLe HX12 CX11 CX21    500.0    97.25 ! Nobs =    1
ANGLe CX13 CX11 CX21    500.0   108.96 ! Nobs =    1
ANGLe CX11 CX13 CX14    500.0   120.05 ! Nobs =    1
ANGLe CX11 CX13 OX77    500.0   121.67 ! Nobs =    1
ANGLe CX14 CX13 OX77    500.0   121.66 ! Nobs =    1
ANGLe CX13 CX14 HX15    500.0   106.36 ! Nobs =    1
ANGLe CX13 CX14 HX16    500.0   106.35 ! Nobs =    1
ANGLe CX13 CX14 CX17    500.0   116.66 ! Nobs =    1
ANGLe HX15 CX14 HX16    500.0   112.39 ! Nobs =    1
ANGLe HX15 CX14 CX17    500.0   104.90 ! Nobs =    1
ANGLe HX16 CX14 CX17    500.0   104.91 ! Nobs =    1
ANGLe CX14 CX17 HX18    500.0   111.14 ! Nobs =    1
ANGLe CX14 CX17 CX19    500.0   111.13 ! Nobs =    1
ANGLe CX14 CX17 CX29    500.0   111.99 ! Nobs =    1
ANGLe HX18 CX17 CX19    500.0   107.77 ! Nobs =    1
ANGLe HX18 CX17 CX29    500.0    99.33 ! Nobs =    1
ANGLe CX19 CX17 CX29    500.0   114.81 ! Nobs =    1
ANGLe CX17 CX19 HX20    500.0   110.99 ! Nobs =    1
ANGLe CX17 CX19 CX21    500.0   110.99 ! Nobs =    1
ANGLe CX17 CX19 CX22    500.0   108.96 ! Nobs =    1
ANGLe HX20 CX19 CX21    500.0   107.91 ! Nobs =    1
ANGLe HX20 CX19 CX22    500.0    97.25 ! Nobs =    1
ANGLe CX21 CX19 CX22    500.0   119.85 ! Nobs =    1
ANGLe CX1  CX21 CX11    500.0   112.44 ! Nobs =    1
ANGLe CX1  CX21 CX19    500.0   109.48 ! Nobs =    1
ANGLe CX1  CX21 CX43    500.0   107.27 ! Nobs =    1
ANGLe CX11 CX21 CX19    500.0   104.36 ! Nobs =    1
ANGLe CX11 CX21 CX43    500.0   107.16 ! Nobs =    1
ANGLe CX19 CX21 CX43    500.0   113.27 ! Nobs =    1
ANGLe CX19 CX22 HX23    500.0   111.45 ! Nobs =    1
ANGLe CX19 CX22 HX24    500.0   111.48 ! Nobs =    1
ANGLe CX19 CX22 CX25    500.0   111.46 ! Nobs =    1
ANGLe HX23 CX22 HX24    500.0   107.40 ! Nobs =    1
ANGLe HX23 CX22 CX25    500.0   107.42 ! Nobs =    1
ANGLe HX24 CX22 CX25    500.0   107.41 ! Nobs =    1
ANGLe CX22 CX25 HX26    500.0   108.40 ! Nobs =    1
ANGLe CX22 CX25 HX27    500.0   108.39 ! Nobs =    1
ANGLe CX22 CX25 CX28    500.0   113.99 ! Nobs =    1
ANGLe HX26 CX25 HX27    500.0   110.54 ! Nobs =    1
ANGLe HX26 CX25 CX28    500.0   107.77 ! Nobs =    1
ANGLe HX27 CX25 CX28    500.0   107.76 ! Nobs =    1
ANGLe CX25 CX28 CX29    500.0   109.13 ! Nobs =    1
ANGLe CX25 CX28 CX37    500.0   111.71 ! Nobs =    1
ANGLe CX25 CX28 CX39    500.0   113.67 ! Nobs =    1
ANGLe CX29 CX28 CX37    500.0   100.39 ! Nobs =    1
ANGLe CX29 CX28 CX39    500.0   110.46 ! Nobs =    1
ANGLe CX37 CX28 CX39    500.0   110.68 ! Nobs =    1
ANGLe CX17 CX29 CX28    500.0   112.70 ! Nobs =    1
ANGLe CX17 CX29 HX30    500.0   112.70 ! Nobs =    1
ANGLe CX17 CX29 CX31    500.0   122.58 ! Nobs =    1
ANGLe CX28 CX29 HX30    500.0   106.05 ! Nobs =    1
ANGLe CX28 CX29 CX31    500.0   106.96 ! Nobs =    1
ANGLe HX30 CX29 CX31    500.0    93.35 ! Nobs =    1
```

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ANGLe CX29 CX31 HX32    500.0   112.94 ! Nobs =    1
ANGLe CX29 CX31 HX33    500.0   112.91 ! Nobs =    1
ANGLe CX29 CX31 CX34    500.0    95.84 ! Nobs =    1
ANGLe HX32 CX31 HX33    500.0   105.81 ! Nobs =    1
ANGLe HX32 CX31 CX34    500.0   114.73 ! Nobs =    1
ANGLe HX33 CX31 CX34    500.0   114.75 ! Nobs =    1
ANGLe CX31 CX34 HX35    500.0   107.31 ! Nobs =    1
ANGLe CX31 CX34 HX36    500.0   107.30 ! Nobs =    1
ANGLe CX31 CX34 CX37    500.0   118.22 ! Nobs =    1
ANGLe HX35 CX34 HX36    500.0   111.55 ! Nobs =    1
ANGLe HX35 CX34 CX37    500.0   106.26 ! Nobs =    1
ANGLe HX36 CX34 CX37    500.0   106.25 ! Nobs =    1
ANGLe CX28 CX37 CX34    500.0    96.08 ! Nobs =    1
ANGLe CX28 CX37 HX38    500.0   112.85 ! Nobs =    1
ANGLe CX28 CX37 CX47    500.0   120.56 ! Nobs =    1
ANGLe CX34 CX37 HX38    500.0   114.67 ! Nobs =    1
ANGLe CX34 CX37 CX47    500.0   119.25 ! Nobs =    1
ANGLe HX38 CX37 CX47    500.0    94.74 ! Nobs =    1
ANGLe CX28 CX39 HX40    500.0   109.49 ! Nobs =    1
ANGLe CX28 CX39 HX41    500.0   109.50 ! Nobs =    1
ANGLe CX28 CX39 HX42    500.0   109.52 ! Nobs =    1
ANGLe HX40 CX39 HX41    500.0   109.45 ! Nobs =    1
ANGLe HX40 CX39 HX42    500.0   109.44 ! Nobs =    1
ANGLe HX41 CX39 HX42    500.0   109.43 ! Nobs =    1
ANGLe CX21 CX43 HX44    500.0   109.50 ! Nobs =    1
ANGLe CX21 CX43 HX45    500.0   109.48 ! Nobs =    1
ANGLe CX21 CX43 HX46    500.0   109.48 ! Nobs =    1
ANGLe HX44 CX43 HX45    500.0   109.45 ! Nobs =    1
ANGLe HX44 CX43 HX46    500.0   109.43 ! Nobs =    1
ANGLe HX45 CX43 HX46    500.0   109.49 ! Nobs =    1
ANGLe CX37 CX47 HX48    500.0   108.16 ! Nobs =    1
ANGLe CX37 CX47 CX49    500.0   114.89 ! Nobs =    1
ANGLe CX37 CX47 CX53    500.0   110.19 ! Nobs =    1
ANGLe HX48 CX47 CX49    500.0   107.43 ! Nobs =    1
ANGLe HX48 CX47 CX53    500.0   100.58 ! Nobs =    1
ANGLe CX49 CX47 CX53    500.0   114.39 ! Nobs =    1
ANGLe CX47 CX49 HX50    500.0   109.48 ! Nobs =    1
ANGLe CX47 CX49 HX51    500.0   109.52 ! Nobs =    1
ANGLe CX47 CX49 HX52    500.0   109.51 ! Nobs =    1
ANGLe HX50 CX49 HX51    500.0   109.43 ! Nobs =    1
ANGLe HX50 CX49 HX52    500.0   109.45 ! Nobs =    1
ANGLe HX51 CX49 HX52    500.0   109.43 ! Nobs =    1
ANGLe CX47 CX53 HX54    500.0   106.32 ! Nobs =    1
ANGLe CX47 CX53 CX55    500.0   122.26 ! Nobs =    1
ANGLe CX47 CX53 OX78    500.0   106.30 ! Nobs =    1
ANGLe HX54 CX53 CX55    500.0   104.82 ! Nobs =    1
ANGLe HX54 CX53 OX78    500.0   112.41 ! Nobs =    1
ANGLe CX55 CX53 OX78    500.0   104.85 ! Nobs =    1
ANGLe CX53 CX55 HX56    500.0   108.06 ! Nobs =    1
ANGLe CX53 CX55 CX57    500.0   115.30 ! Nobs =    1
ANGLe CX53 CX55 OX80    500.0   108.04 ! Nobs =    1
ANGLe HX56 CX55 CX57    500.0   107.29 ! Nobs =    1
ANGLe HX56 CX55 OX80    500.0   110.87 ! Nobs =    1
ANGLe CX57 CX55 OX80    500.0   107.30 ! Nobs =    1
ANGLe CX55 CX57 HX58    500.0   106.03 ! Nobs =    1
ANGLe CX55 CX57 CX59    500.0   123.35 ! Nobs =    1
ANGLe CX55 CX57 CX69    500.0   106.03 ! Nobs =    1
ANGLe HX58 CX57 CX59    500.0   104.45 ! Nobs =    1
ANGLe HX58 CX57 CX69    500.0   112.70 ! Nobs =    1
ANGLe CX59 CX57 CX69    500.0   104.44 ! Nobs =    1
ANGLe CX57 CX59 HX60    500.0   107.97 ! Nobs =    1
```

```
 ANGLe CX57 CX59 CX61    500.0   115.67 ! Nobs =    1
 ANGLe CX57 CX59 CX65    500.0   115.39 ! Nobs =    1
 ANGLe HX60 CX59 CX61    500.0   107.15 ! Nobs =    1
 ANGLe HX60 CX59 CX65    500.0    86.82 ! Nobs =    1
 ANGLe CX61 CX59 CX65    500.0   118.71 ! Nobs =    1
 ANGLe CX59 CX61 HX62    500.0   109.48 ! Nobs =    1
 ANGLe CX59 CX61 HX63    500.0   109.48 ! Nobs =    1
 ANGLe CX59 CX61 HX64    500.0   109.51 ! Nobs =    1
 ANGLe HX62 CX61 HX63    500.0   109.45 ! Nobs =    1
 ANGLe HX62 CX61 HX64    500.0   109.49 ! Nobs =    1
 ANGLe HX63 CX61 HX64    500.0   109.42 ! Nobs =    1
 ANGLe CX59 CX65 HX66    500.0   109.49 ! Nobs =    1
 ANGLe CX59 CX65 HX67    500.0   109.51 ! Nobs =    1
 ANGLe CX59 CX65 HX68    500.0   109.51 ! Nobs =    1
 ANGLe HX66 CX65 HX67    500.0   109.46 ! Nobs =    1
 ANGLe HX66 CX65 HX68    500.0   109.43 ! Nobs =    1
 ANGLe HX67 CX65 HX68    500.0   109.44 ! Nobs =    1
 ANGLe CX57 CX69 HX70    500.0   109.49 ! Nobs =    1
 ANGLe CX57 CX69 HX71    500.0   109.51 ! Nobs =    1
 ANGLe CX57 CX69 HX72    500.0   109.51 ! Nobs =    1
 ANGLe HX70 CX69 HX71    500.0   109.46 ! Nobs =    1
 ANGLe HX70 CX69 HX72    500.0   109.43 ! Nobs =    1
 ANGLe HX71 CX69 HX72    500.0   109.44 ! Nobs =    1
 ANGLe CX4  OX73 HX74    500.0   109.53 ! Nobs =    1
 ANGLe CX6  OX75 HX76    500.0   109.53 ! Nobs =    1
 ANGLe CX53 OX78 HX79    500.0   109.53 ! Nobs =    1
 ANGLe CX55 OX80 HX81    500.0   109.53 ! Nobs =    1

 { edit if necessary }
! >>> NOTE - unusual value for following improper :    41.34 reset to +35.0
 IMPRoper CX1  HX2  HX3  CX4     750.0 0   40.000 ! Nobs =    1 ... Value =
41.337
 IMPRoper CX1  CX4  CX6  HX7     750.0 0  180.000 ! Nobs =    1 ... Value =
179.060
 IMPRoper CX4  CX1  OX73 HX5     750.0 0   35.000 ! Nobs =    1 ... Value =
33.651
 IMPRoper CX6  CX4  OX75 CX8     750.0 0  -35.000 ! Nobs =    1 ... Value =
-36.600
 IMPRoper CX8  CX6  HX9  HX10    750.0 0   35.000 ! Nobs =    1 ... Value =
33.354
 IMPRoper CX11 CX13 HX12 CX8     750.0 0  -35.000 ! Nobs =    1 ... Value =
-36.699
 IMPRoper CX13 CX11 OX77 CX14    750.0 0    0.000 ! Nobs =    1 ... Value =
-0.005
 IMPRoper CX14 CX13 HX15 HX16    750.0 0   35.000 ! Nobs =    1 ... Value =
35.024
 IMPRoper CX17 CX14 HX18 CX19    750.0 0   35.000 ! Nobs =    1 ... Value =
38.108
 IMPRoper CX19 CX17 HX20 CX21    750.0 0  -35.000 ! Nobs =    1 ... Value =
-36.699
 IMPRoper CX21 CX1  CX11 CX19    750.0 0  -35.000 ! Nobs =    1 ... Value =
-36.065
 IMPRoper CX22 CX19 HX23 HX24    750.0 0   35.000 ! Nobs =    1 ... Value =
32.904
 IMPRoper CX25 CX22 HX26 HX27    750.0 0   35.000 ! Nobs =    1 ... Value =
33.245
 IMPRoper CX28 CX25 CX29 CX37    750.0 0  -35.000 ! Nobs =    1 ... Value =
-39.956
 IMPRoper CX28 CX37 CX47 HX48    750.0 0   60.000 ! Nobs =    1 ... Value =
59.410
 IMPRoper CX28 CX37 CX47 CX49    750.0 0  -60.000 ! Nobs =    1 ... Value =
```

```
-60.570
! >>> NOTE - unusual value for following improper :    29.90 reset to +35.0
 IMPRoper CX29 CX17 CX28 HX30    750.0 0   35.000 ! Nobs =    1 ... Value =
29.898
 IMPRoper CX31 CX29 HX32 HX33    750.0 0   35.000 ! Nobs =    1 ... Value =
33.012
 IMPRoper CX34 CX31 HX35 HX36    750.0 0   35.000 ! Nobs =    1 ... Value =
33.715
! >>> NOTE - unusual value for following improper :   -27.26 reset to -35.0
 IMPRoper CX37 CX28 CX34 HX38    750.0 0  -30.000 ! Nobs =    1 ... Value =
-27.264
 IMPRoper CX39 CX28 HX40 HX41    750.0 0  -35.000 ! Nobs =    1 ... Value =
-33.155
 IMPRoper CX43 CX21 HX44 HX45    750.0 0  -35.000 ! Nobs =    1 ... Value =
-33.101
 IMPRoper CX47 CX37 HX48 CX49    750.0 0   35.000 ! Nobs =    1 ... Value =
35.534
 IMPRoper CX49 CX47 HX50 HX51    750.0 0  -35.000 ! Nobs =    1 ... Value =
-33.451
 IMPRoper CX53 CX47 OX78 HX54    750.0 0   35.000 ! Nobs =    1 ... Value =
33.694
 IMPRoper CX55 CX53 HX56 OX80    750.0 0   35.000 ! Nobs =    1 ... Value =
33.587
 IMPRoper CX57 CX55 CX69 HX58    750.0 0   35.000 ! Nobs =    1 ... Value =
33.806
 IMPRoper CX59 CX57 HX60 CX61    750.0 0   35.000 ! Nobs =    1 ... Value =
35.219
 IMPRoper CX61 CX59 HX62 HX63    750.0 0  -35.000 ! Nobs =    1 ... Value =
-33.482
 IMPRoper CX65 CX59 HX66 HX67    750.0 0  -35.000 ! Nobs =    1 ... Value =
-33.434
 IMPRoper CX69 CX57 HX70 HX71    750.0 0  -35.000 ! Nobs =    1 ... Value =
-33.434

 { edit if necessary }
 NONBonded CX1  0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX2  0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX3  0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX4  0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX5  0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX6  0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX7  0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX8  0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX9  0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX10 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX11 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX12 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX13 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded CX14 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX15 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX16 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX17 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX18 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX19 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX20 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX21 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded CX22 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX23 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX24 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX25 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX26 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
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```
 NONBonded HX27 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX28 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded CX29 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX30 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX31 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX32 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX33 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX34 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX35 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX36 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX37 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX38 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX39 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX40 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX41 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX42 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX43 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX44 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX45 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX46 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX47 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX48 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX49 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX50 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX51 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX52 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX53 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX54 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX55 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX56 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX57 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX58 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX59 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX60 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX61 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX62 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX63 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX64 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX65 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX66 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX67 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX68 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX69 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX70 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX71 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX72 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded OX73 0.1591  2.8509    0.1591  2.8509 ! assuming Oxygen
 NONBonded HX74 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded OX75 0.1591  2.8509    0.1591  2.8509 ! assuming Oxygen
 NONBonded HX76 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded OX77 0.1591  2.8509    0.1591  2.8509 ! assuming Oxygen
 NONBonded OX78 0.1591  2.8509    0.1591  2.8509 ! assuming Oxygen
 NONBonded HX79 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded OX80 0.1591  2.8509    0.1591  2.8509 ! assuming Oxygen
 NONBonded HX81 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen

 set echo=true end
```

DHO_par.txt

```
Remarks ../../tmp/hicup_btcpxq_9551/DHO_top.txt
Remarks Created by XPLO2D V. 001221/2.8.9 at Wed Aug 29 16:04:45 2001 for
A. Nonymous
Remarks Auto-generated by XPLO2D from file ../../tmp/hicup_btcpxq_
9551/user.pdb
Remarks You *MUST* check/edit MASSes and CHARges !!!
Remarks Check DONOrs and ACCEptors
Remarks Verify IMPRopers yourself
Remarks DIHEdrals which are not flat are commented out

 set echo=false end

 { edit masses if necessary }
 MASS CX1    12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX2     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX3     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX4    12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX5     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX6     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX7    12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX8     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX9    12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX10    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX11    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX12   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX13    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX14   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX15    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX16    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX17   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX18    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX19    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX20   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX21    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX22   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX23    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX24   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS CX25   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX26    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX27    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX28   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX29    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX30   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS CX31   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX32    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX33   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX34    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX35    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX36   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX37    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX38    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX39   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX40    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX41   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX42    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX43    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX44    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX45   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX46    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX47    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX48    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
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 MASS CX49   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX50    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX51   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX52    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX53    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX54    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX55   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX56    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX57    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX58   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX59    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX60    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX61   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS OX62   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
 MASS HX63    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS OX64   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
 MASS HX65    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS OX66   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
 MASS OX67   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)

 autogenerate angles=true end

RESIdue DHO

GROUp
 ATOM  C1   TYPE CX1   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H11  TYPE HX2   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H12  TYPE HX3   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C2   TYPE CX4   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H21  TYPE HX5   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H22  TYPE HX6   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C3   TYPE CX7   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H3   TYPE HX8   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C4   TYPE CX9   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H41  TYPE HX10  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H42  TYPE HX11  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C5   TYPE CX12  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H5   TYPE HX13  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C6   TYPE CX14  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H61  TYPE HX15  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H62  TYPE HX16  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C7   TYPE CX17  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H71  TYPE HX18  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H72  TYPE HX19  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C8   TYPE CX20  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H8   TYPE HX21  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C9   TYPE CX22  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H9   TYPE HX23  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C10  TYPE CX24  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C11  TYPE CX25  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H111  TYPE HX26  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H112  TYPE HX27  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C12  TYPE CX28  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H121  TYPE HX29  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C13  TYPE CX30  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C14  TYPE CX31  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H14  TYPE HX32  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C15  TYPE CX33  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H151  TYPE HX34  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H152  TYPE HX35  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C16  TYPE CX36  CHARge  0.0  END ! Nr of Hs =  0
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ATOM H161  TYPE HX37  CHARge  0.0  END ! Nr of Hs =  0
ATOM H162  TYPE HX38  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C17  TYPE CX39  CHARge  0.0  END ! Nr of Hs =  0
ATOM  H17  TYPE HX40  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C18  TYPE CX41  CHARge  0.0  END ! Nr of Hs =  0
ATOM H181  TYPE HX42  CHARge  0.0  END ! Nr of Hs =  0
ATOM H182  TYPE HX43  CHARge  0.0  END ! Nr of Hs =  0
ATOM H183  TYPE HX44  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C19  TYPE CX45  CHARge  0.0  END ! Nr of Hs =  0
ATOM H191  TYPE HX46  CHARge  0.0  END ! Nr of Hs =  0
ATOM H192  TYPE HX47  CHARge  0.0  END ! Nr of Hs =  0
ATOM H193  TYPE HX48  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C20  TYPE CX49  CHARge  0.0  END ! Nr of Hs =  0
ATOM  H20  TYPE HX50  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C21  TYPE CX51  CHARge  0.0  END ! Nr of Hs =  0
ATOM H211  TYPE HX52  CHARge  0.0  END ! Nr of Hs =  0
ATOM H212  TYPE HX53  CHARge  0.0  END ! Nr of Hs =  0
ATOM H213  TYPE HX54  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C22  TYPE CX55  CHARge  0.0  END ! Nr of Hs =  0
ATOM H221  TYPE HX56  CHARge  0.0  END ! Nr of Hs =  0
ATOM H222  TYPE HX57  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C23  TYPE CX58  CHARge  0.0  END ! Nr of Hs =  0
ATOM H231  TYPE HX59  CHARge  0.0  END ! Nr of Hs =  0
ATOM H232  TYPE HX60  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C24  TYPE CX61  CHARge  0.0  END ! Nr of Hs =  0
ATOM  O1   TYPE OX62  CHARge  0.0  END ! Nr of Hs =  0
ATOM  H1   TYPE HX63  CHARge  0.0  END ! Nr of Hs =  0
ATOM  O2   TYPE OX64  CHARge  0.0  END ! Nr of Hs =  0
ATOM  H2   TYPE HX65  CHARge  0.0  END ! Nr of Hs =  0
ATOM  O3   TYPE OX66  CHARge  0.0  END ! Nr of Hs =  0
ATOM  O4   TYPE OX67  CHARge  0.0  END ! Nr of Hs =  0

BOND  C1   H11      BOND  C1   H12      BOND  C1   C2       BOND  C1   C10
BOND  C2   H21      BOND  C2   H22      BOND  C2   C3       BOND  C3   H3
BOND  C3   C4       BOND  C3   O1       BOND  C4   H41      BOND  C4   H42
BOND  C4   C5       BOND  C5   H5       BOND  C5   C6       BOND  C5   C10
BOND  C6   H61      BOND  C6   H62      BOND  C6   C7       BOND  C7   H71
BOND  C7   H72      BOND  C7   C8       BOND  C8   H8       BOND  C8   C9
BOND  C8   C14      BOND  C9   H9       BOND  C9   C10      BOND  C9   C11
BOND  C10  C19      BOND  C11 H111      BOND  C11 H112      BOND  C11  C12
BOND  C12 H121      BOND  C12  C13      BOND  C12  O2       BOND  C13  C14
BOND  C13  C17      BOND  C13  C18      BOND  C14  H14      BOND  C14  C15
BOND  C15 H151      BOND  C15 H152      BOND  C15  C16      BOND  C16 H161
BOND  C16 H162      BOND  C16  C17      BOND  C17  H17      BOND  C17  C20
BOND  C18 H181      BOND  C18 H182      BOND  C18 H183      BOND  C19 H191
BOND  C19 H192      BOND  C19 H193      BOND  C20  H20      BOND  C20  C21
BOND  C20  C22      BOND  C21 H211      BOND  C21 H212      BOND  C21 H213
BOND  C22 H221      BOND  C22 H222      BOND  C22  C23      BOND  C23 H231
BOND  C23 H232      BOND  C23  C24      BOND  C24  O3       BOND  C24  O4
BOND  O1   H1       BOND  O2   H2

 { edit these DIHEdrals if necessary }
! DIHEdral  H11  C1   C2   H21 ! flat ? (180 degrees = trans)   180.64
! DIHEdral  H11  C1   C2   H22 ! flexible dihedral ???    60.64
! DIHEdral  H11  C1   C2   C3  ! flexible dihedral ???   -59.34
! DIHEdral  H12  C1   C2   H21 ! flexible dihedral ???    60.64
! DIHEdral  H12  C1   C2   H22 ! flexible dihedral ???   -59.36
! DIHEdral  H12  C1   C2   C3  ! flat ? (180 degrees = trans)   180.66
! DIHEdral  C10  C1   C2   H21 ! flexible dihedral ???   -59.35
! DIHEdral  C10  C1   C2   H22 ! flat ? (180 degrees = trans)   180.65
! DIHEdral  C10  C1   C2   C3  ! flexible dihedral ???    60.67
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! DIHEdral  H11  C1   C10  C5  ! flexible dihedral ???    61.65
! DIHEdral  H11  C1   C10  C9  ! flat ? (180 degrees = trans)   181.19
! DIHEdral  H11  C1   C10  C19 ! flexible dihedral ???   -58.28
! DIHEdral  H12  C1   C10  C5  ! flat ? (180 degrees = trans)   180.75
! DIHEdral  H12  C1   C10  C9  ! flexible dihedral ???   -59.71
! DIHEdral  H12  C1   C10  C19 ! flexible dihedral ???    60.82
! DIHEdral  C2   C1   C10  C5  ! flexible dihedral ???   -58.81
! DIHEdral  C2   C1   C10  C9  ! flexible dihedral ???    60.73
! DIHEdral  C2   C1   C10  C19 ! flat ? (180 degrees = trans)   181.26
! DIHEdral  C1   C2   C3   H3  ! flexible dihedral ???    60.48
! DIHEdral  C1   C2   C3   C4  ! flexible dihedral ???   -59.11
! DIHEdral  C1   C2   C3   O1  ! flat ? (180 degrees = trans)   180.48
! DIHEdral  H21  C2   C3   H3  ! flat ? (180 degrees = trans)   177.15
! DIHEdral  H21  C2   C3   C4  ! flexible dihedral ???    57.56
! DIHEdral  H21  C2   C3   O1  ! flexible dihedral ???   -62.85
! DIHEdral  H22  C2   C3   H3  ! flexible dihedral ???   -56.17
! DIHEdral  H22  C2   C3   C4  ! flat ? (180 degrees = trans)   184.24
! DIHEdral  H22  C2   C3   O1  ! flexible dihedral ???    63.83
! DIHEdral  C2   C3   C4   H41 ! flexible dihedral ???   -60.08
! DIHEdral  C2   C3   C4   H42 ! flat ? (180 degrees = trans)   179.96
! DIHEdral  C2   C3   C4   C5  ! flexible dihedral ???    59.93
! DIHEdral  H3   C3   C4   H41 ! flat ? (180 degrees = trans)   180.00
! DIHEdral  H3   C3   C4   H42 ! flexible dihedral ???    60.04
! DIHEdral  H3   C3   C4   C5  ! flexible dihedral ???   -59.99
! DIHEdral  O1   C3   C4   H41 ! flexible dihedral ???    60.26
! DIHEdral  O1   C3   C4   H42 ! flexible dihedral ???   -59.70
! DIHEdral  O1   C3   C4   C5  ! flat ? (180 degrees = trans)   180.27
! DIHEdral  C2   C3   O1   H1  ! flexible dihedral ???   -50.93
! DIHEdral  H3   C3   O1   H1  ! flexible dihedral ???    69.22
! DIHEdral  C4   C3   O1   H1  ! flat ? (180 degrees = trans)   188.77
! DIHEdral  C3   C4   C5   H5  ! flexible dihedral ???    57.98
! DIHEdral  C3   C4   C5   C6  ! flat ? (180 degrees = trans)   177.97
! DIHEdral  C3   C4   C5   C10 ! flexible dihedral ???   -57.95
! DIHEdral  H41  C4   C5   H5  ! flat ? (180 degrees = trans)   178.78
! DIHEdral  H41  C4   C5   C6  ! flexible dihedral ???   -61.23
! DIHEdral  H41  C4   C5   C10 ! flexible dihedral ???    62.86
! DIHEdral  H42  C4   C5   H5  ! flexible dihedral ???   -62.82
! DIHEdral  H42  C4   C5   C6  ! flexible dihedral ???    57.16
! DIHEdral  H42  C4   C5   C10 ! flat ? (180 degrees = trans)   181.25
! DIHEdral  C4   C5   C6   H61 ! flexible dihedral ???   -54.20
! DIHEdral  C4   C5   C6   H62 ! flat ? (180 degrees = trans)   185.79
! DIHEdral  C4   C5   C6   C7  ! flexible dihedral ???    65.79
! DIHEdral  H5   C5   C6   H61 ! flexible dihedral ???    69.97
! DIHEdral  H5   C5   C6   H62 ! flexible dihedral ???   -50.04
! DIHEdral  H5   C5   C6   C7  ! flat ? (180 degrees = trans)   189.95
! DIHEdral  C10  C5   C6   H61 ! flat ? (180 degrees = trans)   181.66
! DIHEdral  C10  C5   C6   H62 ! flexible dihedral ???    61.65
! DIHEdral  C10  C5   C6   C7  ! flexible dihedral ???   -58.36
! DIHEdral  C4   C5   C10  C1  ! flexible dihedral ???    54.29
! DIHEdral  C4   C5   C10  C9  ! flexible dihedral ???   -67.83
! DIHEdral  C4   C5   C10  C19 ! flat ? (180 degrees = trans)   172.83
! DIHEdral  H5   C5   C10  C1  ! flexible dihedral ???   -67.25
! DIHEdral  H5   C5   C10  C9  ! flat ? (180 degrees = trans)   170.64
! DIHEdral  H5   C5   C10  C19 ! flexible dihedral ???    51.30
! DIHEdral  C6   C5   C10  C1  ! flat ? (180 degrees = trans)   179.95
! DIHEdral  C6   C5   C10  C9  ! flexible dihedral ???    57.83
! DIHEdral  C6   C5   C10  C19 ! flexible dihedral ???   -61.51
! DIHEdral  C5   C6   C7   H71 ! flexible dihedral ???   -60.18
! DIHEdral  C5   C6   C7   H72 ! flat ? (180 degrees = trans)   179.83
! DIHEdral  C5   C6   C7   C8  ! flexible dihedral ???    59.83
! DIHEdral  H61  C6   C7   H71 ! flexible dihedral ???    61.35
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! DIHEdral  H61  C6   C7   H72 ! flexible dihedral ???   -58.64
! DIHEdral  H61  C6   C7   C8  ! flat ? (180 degrees = trans)   181.36
! DIHEdral  H62  C6   C7   H71 ! flat ? (180 degrees = trans)   178.27
! DIHEdral  H62  C6   C7   H72 ! flexible dihedral ???    58.28
! DIHEdral  H62  C6   C7   C8  ! flexible dihedral ???   -61.72
! DIHEdral  C6   C7   C8   H8  ! flexible dihedral ???    60.70
! DIHEdral  C6   C7   C8   C9  ! flexible dihedral ???   -59.29
! DIHEdral  C6   C7   C8   C14 ! flat ? (180 degrees = trans)   180.70
! DIHEdral  H71  C7   C8   H8  ! flat ? (180 degrees = trans)   183.70
! DIHEdral  H71  C7   C8   C9  ! flexible dihedral ???    63.70
! DIHEdral  H71  C7   C8   C14 ! flexible dihedral ???   -56.30
! DIHEdral  H72  C7   C8   H8  ! flexible dihedral ???   -62.28
! DIHEdral  H72  C7   C8   C9  ! flat ? (180 degrees = trans)   177.72
! DIHEdral  H72  C7   C8   C14 ! flexible dihedral ???    57.72
! DIHEdral  C7   C8   C9   H9  ! flexible dihedral ???   -60.83
! DIHEdral  C7   C8   C9   C10 ! flexible dihedral ???    59.17
! DIHEdral  C7   C8   C9   C11 ! flat ? (180 degrees = trans)   181.00
! DIHEdral  H8   C8   C9   H9  ! flat ? (180 degrees = trans)   181.80
! DIHEdral  H8   C8   C9   C10 ! flexible dihedral ???   -58.20
! DIHEdral  H8   C8   C9   C11 ! flexible dihedral ???    63.62
! DIHEdral  C14  C8   C9   H9  ! flexible dihedral ???    61.20
! DIHEdral  C14  C8   C9   C10 ! flat ? (180 degrees = trans)   181.20
! DIHEdral  C14  C8   C9   C11 ! flexible dihedral ???   -56.98
! DIHEdral  C7   C8   C14  C13 ! flat ? (180 degrees = trans)   179.12
! DIHEdral  C7   C8   C14  H14 ! flexible dihedral ???    59.10
! DIHEdral  C7   C8   C14  C15 ! flexible dihedral ???   -59.80
! DIHEdral  H8   C8   C14  C13 ! flexible dihedral ???   -61.90
! DIHEdral  H8   C8   C14  H14 ! flat ? (180 degrees = trans)   178.08
! DIHEdral  H8   C8   C14  C15 ! flexible dihedral ???    59.18
! DIHEdral  C9   C8   C14  C13 ! flexible dihedral ???    60.12
! DIHEdral  C9   C8   C14  H14 ! flexible dihedral ???   -59.90
! DIHEdral  C9   C8   C14  C15 ! flat ? (180 degrees = trans)   181.20
! DIHEdral  C8   C9   C10  C1  ! flat ? (180 degrees = trans)   181.41
! DIHEdral  C8   C9   C10  C5  ! flexible dihedral ???   -59.37
! DIHEdral  C8   C9   C10  C19 ! flexible dihedral ???    61.09
! DIHEdral  H9   C9   C10  C1  ! flexible dihedral ???   -57.43
! DIHEdral  H9   C9   C10  C5  ! flexible dihedral ???    61.80
! DIHEdral  H9   C9   C10  C19 ! flat ? (180 degrees = trans)   182.26
! DIHEdral  C11  C9   C10  C1  ! flexible dihedral ???    60.90
! DIHEdral  C11  C9   C10  C5  ! flat ? (180 degrees = trans)   180.13
! DIHEdral  C11  C9   C10  C19 ! flexible dihedral ???   -59.41
! DIHEdral  C8   C9   C11 H111 ! flexible dihedral ???   -61.63
! DIHEdral  C8   C9   C11 H112 ! flat ? (180 degrees = trans)   178.40
! DIHEdral  C8   C9   C11  C12 ! flexible dihedral ???    58.41
! DIHEdral  H9   C9   C11 H111 ! flat ? (180 degrees = trans)   178.61
! DIHEdral  H9   C9   C11 H112 ! flexible dihedral ???    58.64
! DIHEdral  H9   C9   C11  C12 ! flexible dihedral ???   -61.36
! DIHEdral  C10  C9   C11 H111 ! flexible dihedral ???    59.94
! DIHEdral  C10  C9   C11 H112 ! flexible dihedral ???   -60.03
! DIHEdral  C10  C9   C11  C12 ! flat ? (180 degrees = trans)   179.97
! DIHEdral  C1   C10  C19 H191 ! flat ? (0 degrees = cis)     0.00
! DIHEdral  C5   C10  C19 H192 ! flat ? (0 degrees = cis)     1.84
! DIHEdral  C9   C10  C19 H193 ! flat ? (0 degrees = cis)     2.78
! DIHEdral  C9   C11  C12 H121 ! flat ? (180 degrees = trans)   179.49
! DIHEdral  C9   C11  C12  C13 ! flexible dihedral ???   -60.79
! DIHEdral  C9   C11  C12  O2  ! flexible dihedral ???    59.49
! DIHEdral H111  C11  C12 H121 ! flexible dihedral ???   -58.55
! DIHEdral H111  C11  C12  C13 ! flexible dihedral ???    61.16
! DIHEdral H111  C11  C12  O2  ! flat ? (180 degrees = trans)   181.45
! DIHEdral H112  C11  C12 H121 ! flexible dihedral ???    57.55
! DIHEdral H112  C11  C12  C13 ! flat ? (180 degrees = trans)   177.27
```

```
! DIHEdral H112  C11  C12  O2  ! flexible dihedral ???   -62.45
! DIHEdral  C11  C12  C13  C14 ! flexible dihedral ???    57.69
! DIHEdral  C11  C12  C13  C18 ! flexible dihedral ???   -60.01
! DIHEdral H121  C12  C13  C14 ! flat ? (180 degrees = trans)   178.36
! DIHEdral H121  C12  C13  C18 ! flexible dihedral ???    60.66
! DIHEdral  O2   C12  C13  C14 ! flexible dihedral ???   -63.27
! DIHEdral  O2   C12  C13  C18 ! flat ? (180 degrees = trans)   179.03
! DIHEdral  C12  C13  C14  C8  ! flexible dihedral ???   -59.72
! DIHEdral  C12  C13  C14  H14 ! flexible dihedral ???    60.64
! DIHEdral  C12  C13  C14  C15 ! flat ? (180 degrees = trans)   172.08
! DIHEdral  C17  C13  C14  C8  ! flat ? (180 degrees = trans)   177.13
! DIHEdral  C17  C13  C14  H14 ! flexible dihedral ???   -62.51
! DIHEdral  C18  C13  C14  C8  ! flexible dihedral ???    59.76
! DIHEdral  C18  C13  C14  H14 ! flat ? (180 degrees = trans)   180.12
! DIHEdral  C18  C13  C14  C15 ! flexible dihedral ???   -68.44
! DIHEdral  C14  C13  C17  C20 ! flat ? (180 degrees = trans)   189.18
! DIHEdral  C18  C13  C17  C16 ! flexible dihedral ???    69.81
! DIHEdral  C18  C13  C17  H17 ! flat ? (180 degrees = trans)   189.82
! DIHEdral  C18  C13  C17  C20 ! flexible dihedral ???   -56.80
! DIHEdral  C12  C13  C18 H181 ! flat ? (0 degrees = cis)     0.00
! DIHEdral  C14  C13  C18 H182 ! flat ? (0 degrees = cis)     3.74
! DIHEdral  C13  C14  C15 H152 ! flexible dihedral ???    86.33
! DIHEdral  C14  C15  C16  C17 ! flat ? (0 degrees = cis)     5.80
! DIHEdral H151  C15  C16 H161 ! flat ? (0 degrees = cis)     5.25
! DIHEdral H152  C15  C16 H162 ! flat ? (0 degrees = cis)     6.32
! DIHEdral  C15  C16  C17  H17 ! flexible dihedral ???   -94.45
! DIHEdral H161  C16  C17  C20 ! flexible dihedral ???   -89.61
! DIHEdral H162  C16  C17  C13 ! flexible dihedral ???   -91.38
! DIHEdral  C13  C17  C20  H20 ! flexible dihedral ???    66.67
! DIHEdral  C13  C17  C20  C21 ! flexible dihedral ???   -53.35
! DIHEdral  C13  C17  C20  C22 ! flat ? (180 degrees = trans)   180.53
! DIHEdral  C16  C17  C20  H20 ! flexible dihedral ???   -54.79
! DIHEdral  C16  C17  C20  C21 ! flat ? (180 degrees = trans)   185.19
! DIHEdral  C16  C17  C20  C22 ! flexible dihedral ???    59.07
! DIHEdral  H17  C17  C20  H20 ! flat ? (180 degrees = trans)   186.35
! DIHEdral  H17  C17  C20  C21 ! flexible dihedral ???    66.33
! DIHEdral  H17  C17  C20  C22 ! flexible dihedral ???   -59.79
! DIHEdral  C17  C20  C21 H211 ! flat ? (0 degrees = cis)     0.00
! DIHEdral  H20  C20  C21 H212 ! flat ? (0 degrees = cis)    -0.64
! DIHEdral  C22  C20  C21 H213 ! flat ? (0 degrees = cis)     6.45
! DIHEdral  C17  C20  C22 H221 ! flexible dihedral ???   -52.16
! DIHEdral  C17  C20  C22 H222 ! flat ? (180 degrees = trans)   187.88
! DIHEdral  C17  C20  C22  C23 ! flexible dihedral ???    67.87
! DIHEdral  H20  C20  C22 H221 ! flexible dihedral ???    62.67
! DIHEdral  H20  C20  C22 H222 ! flexible dihedral ???   -57.30
! DIHEdral  H20  C20  C22  C23 ! flat ? (180 degrees = trans)   182.70
! DIHEdral  C21  C20  C22 H221 ! flat ? (180 degrees = trans)   175.79
! DIHEdral  C21  C20  C22 H222 ! flexible dihedral ???    55.82
! DIHEdral  C21  C20  C22  C23 ! flexible dihedral ???   -64.18
! DIHEdral  C20  C22  C23 H231 ! flexible dihedral ???    51.62
! DIHEdral  C20  C22  C23 H232 ! flexible dihedral ???   -68.36
! DIHEdral  C20  C22  C23  C24 ! flat ? (180 degrees = trans)   171.63
! DIHEdral H221  C22  C23 H231 ! flat ? (180 degrees = trans)   172.08
! DIHEdral H221  C22  C23 H232 ! flexible dihedral ???    52.10
! DIHEdral H221  C22  C23  C24 ! flexible dihedral ???   -67.91
! DIHEdral H222  C22  C23 H231 ! flexible dihedral ???   -68.83
! DIHEdral H222  C22  C23 H232 ! flat ? (180 degrees = trans)   171.19
! DIHEdral H222  C22  C23  C24 ! flexible dihedral ???    51.18
! DIHEdral  C22  C23  C24  O3  ! flat ? (0 degrees = cis)    -8.50
! DIHEdral  C22  C23  C24  O4  ! flat ? (180 degrees = trans)   171.64
! DIHEdral H231  C23  C24  O4  ! flexible dihedral ???   -64.92
```

```
 { edit these IMPRopers if necessary }
 IMPRoper  C1   H11  H12  C2  ! chirality or flatness improper    41.49
 IMPRoper  C1   C2   C3   O1  ! dihedral improper               180.48
 IMPRoper  C2   C1   H21  H22 ! chirality or flatness improper    33.57
 IMPRoper  C3   C2   H3   C4  ! chirality or flatness improper    37.92
 IMPRoper  C3   C4   C5   C6  ! dihedral improper               177.97
 IMPRoper  C4   C3   H41  H42 ! chirality or flatness improper    33.25
 IMPRoper  C5   C4   H5   C6  ! chirality or flatness improper   -37.38
 IMPRoper  C6   C5   H61  H62 ! chirality or flatness improper    33.12
 IMPRoper  C7   C6   H71  H72 ! chirality or flatness improper    32.97
 IMPRoper  C8   C7   H8   C9  ! chirality or flatness improper    38.50
 IMPRoper  C9   C8   H9   C10 ! chirality or flatness improper   -38.36
 IMPRoper  C10  C1   C5   C9  ! chirality or flatness improper   -34.83
 IMPRoper  C11  C9  H111 H112 ! chirality or flatness improper    33.05
 IMPRoper  C12  C11 H121  C13 ! chirality or flatness improper   -38.06
 IMPRoper  C13  C12  C14  C17 ! chirality or flatness improper   -36.07
! IMPRoper  C13  C17  C20  H20 ! dihedral improper                66.67
! IMPRoper  C13  C17  C20  C21 ! dihedral improper               -53.35
 IMPRoper  C14  C8   C13  H14 ! chirality or flatness improper    31.42
 IMPRoper  C15  C14 H151 H152 ! chirality or flatness improper    33.07
 IMPRoper  C16  C15 H161 H162 ! chirality or flatness improper    33.47
 IMPRoper  C17  C13  C16  H17 ! chirality or flatness improper   -28.84
 IMPRoper  C18  C13 H181 H182 ! chirality or flatness improper   -33.05
 IMPRoper  C19  C10 H191 H192 ! chirality or flatness improper   -33.22
 IMPRoper  C20  C17  H20  C21 ! chirality or flatness improper    33.61
 IMPRoper  C21  C20 H211 H212 ! chirality or flatness improper   -33.49
 IMPRoper  C22  C20 H221 H222 ! chirality or flatness improper    33.34
 IMPRoper  C23  C22 H231 H232 ! chirality or flatness improper    33.06
 IMPRoper  C24  C23  O3   O4  ! chirality or flatness improper     0.08

 { edit any DONOrs and ACCEptors if necessary }
 ACCEptor  O1   C3
 ACCEptor  O2   C12
 ACCEptor  O3   C24
 ACCEptor  O4   C24

END { RESIdue DHO }



DHO_top.txt
Remarks ../../tmp/hicup_btcpxq_9551/DHO_top.txt
Remarks Created by XPLO2D V. 001221/2.8.9 at Wed Aug 29 16:04:45 2001 for
A. Nonymous
Remarks Auto-generated by XPLO2D from file ../../tmp/hicup_btcpxq_
9551/user.pdb
Remarks You *MUST* check/edit MASSes and CHARges !!!
Remarks Check DONOrs and ACCEptors
Remarks Verify IMPRopers yourself
Remarks DIHEdrals which are not flat are commented out

 set echo=false end

 { edit masses if necessary }
 MASS CX1    12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX2     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX3     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX4    12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX5     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX6     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
```

```
MASS CX7    12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX8     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX9    12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX10    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX11    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX12   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX13    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX14   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX15    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX16    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX17   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX18    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX19    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX20   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX21    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX22   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX23    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX24   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS CX25   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX26    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX27    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX28   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX29    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX30   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS CX31   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX32    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX33   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX34    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX35    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX36   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX37    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX38    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX39   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX40    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX41   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX42    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX43    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX44    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX45   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX46    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX47    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX48    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX49   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX50    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX51   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX52    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX53    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX54    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX55   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX56    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX57    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX58   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX59    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX60    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX61   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS OX62   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
MASS HX63    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS OX64   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
MASS HX65    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS OX66   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
MASS OX67   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
```

```
 autogenerate angles=true end

RESIdue DHO

GROUp
 ATOM  C1   TYPE CX1   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H11  TYPE HX2   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H12  TYPE HX3   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C2   TYPE CX4   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H21  TYPE HX5   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H22  TYPE HX6   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C3   TYPE CX7   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H3   TYPE HX8   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C4   TYPE CX9   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H41  TYPE HX10  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H42  TYPE HX11  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C5   TYPE CX12  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H5   TYPE HX13  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C6   TYPE CX14  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H61  TYPE HX15  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H62  TYPE HX16  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C7   TYPE CX17  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H71  TYPE HX18  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H72  TYPE HX19  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C8   TYPE CX20  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H8   TYPE HX21  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C9   TYPE CX22  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H9   TYPE HX23  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C10  TYPE CX24  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C11  TYPE CX25  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H111  TYPE HX26  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H112  TYPE HX27  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C12  TYPE CX28  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H121  TYPE HX29  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C13  TYPE CX30  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C14  TYPE CX31  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H14  TYPE HX32  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C15  TYPE CX33  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H151  TYPE HX34  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H152  TYPE HX35  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C16  TYPE CX36  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H161  TYPE HX37  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H162  TYPE HX38  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C17  TYPE CX39  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H17  TYPE HX40  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C18  TYPE CX41  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H181  TYPE HX42  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H182  TYPE HX43  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H183  TYPE HX44  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C19  TYPE CX45  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H191  TYPE HX46  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H192  TYPE HX47  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H193  TYPE HX48  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C20  TYPE CX49  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H20  TYPE HX50  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C21  TYPE CX51  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H211  TYPE HX52  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H212  TYPE HX53  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H213  TYPE HX54  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C22  TYPE CX55  CHARge  0.0  END ! Nr of Hs =  0
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ATOM H221  TYPE HX56  CHARge  0.0  END ! Nr of Hs =  0
ATOM H222  TYPE HX57  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C23  TYPE CX58  CHARge  0.0  END ! Nr of Hs =  0
ATOM H231  TYPE HX59  CHARge  0.0  END ! Nr of Hs =  0
ATOM H232  TYPE HX60  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C24  TYPE CX61  CHARge  0.0  END ! Nr of Hs =  0
ATOM  O1   TYPE OX62  CHARge  0.0  END ! Nr of Hs =  0
ATOM  H1   TYPE HX63  CHARge  0.0  END ! Nr of Hs =  0
ATOM  O2   TYPE OX64  CHARge  0.0  END ! Nr of Hs =  0
ATOM  H2   TYPE HX65  CHARge  0.0  END ! Nr of Hs =  0
ATOM  O3   TYPE OX66  CHARge  0.0  END ! Nr of Hs =  0
ATOM  O4   TYPE OX67  CHARge  0.0  END ! Nr of Hs =  0

BOND  C1   H11       BOND  C1   H12       BOND  C1   C2       BOND  C1   C10
BOND  C2   H21       BOND  C2   H22       BOND  C2   C3       BOND  C3   H3
BOND  C3   C4        BOND  C3   O1        BOND  C4   H41      BOND  C4   H42
BOND  C4   C5        BOND  C5   H5        BOND  C5   C6       BOND  C5   C10
BOND  C6   H61       BOND  C6   H62       BOND  C6   C7       BOND  C7   H71
BOND  C7   H72       BOND  C7   C8        BOND  C8   H8       BOND  C8   C9
BOND  C8   C14       BOND  C9   H9        BOND  C9   C10      BOND  C9   C11
BOND  C10  C19       BOND  C11 H111       BOND  C11 H112       BOND  C11  C12
BOND  C12 H121       BOND  C12  C13       BOND  C12  O2        BOND  C13  C14
BOND  C13  C17       BOND  C13  C18       BOND  C14  H14       BOND  C14  C15
BOND  C15 H151       BOND  C15 H152       BOND  C15  C16       BOND  C16 H161
BOND  C16 H162       BOND  C16  C17       BOND  C17  H17       BOND  C17  C20
BOND  C18 H181       BOND  C18 H182       BOND  C18 H183       BOND  C19 H191
BOND  C19 H192       BOND  C19 H193       BOND  C20  H20       BOND  C20  C21
BOND  C20  C22       BOND  C21 H211       BOND  C21 H212       BOND  C21 H213
BOND  C22 H221       BOND  C22 H222       BOND  C22  C23       BOND  C23 H231
BOND  C23 H232       BOND  C23  C24       BOND  C24  O3        BOND  C24  O4
BOND  O1   H1        BOND  O2   H2

 { edit these DIHEdrals if necessary }
! DIHEdral  H11  C1   C2   H21 ! flat ? (180 degrees = trans)   180.64
! DIHEdral  H11  C1   C2   H22 ! flexible dihedral ???    60.64
! DIHEdral  H11  C1   C2   C3  ! flexible dihedral ???   -59.34
! DIHEdral  H12  C1   C2   H21 ! flexible dihedral ???    60.64
! DIHEdral  H12  C1   C2   H22 ! flexible dihedral ???   -59.36
! DIHEdral  H12  C1   C2   C3  ! flat ? (180 degrees = trans)   180.66
! DIHEdral  C10  C1   C2   H21 ! flexible dihedral ???   -59.35
! DIHEdral  C10  C1   C2   H22 ! flat ? (180 degrees = trans)   180.65
! DIHEdral  C10  C1   C2   C3  ! flexible dihedral ???    60.67
! DIHEdral  H11  C1   C10  C5  ! flexible dihedral ???    61.65
! DIHEdral  H11  C1   C10  C9  ! flat ? (180 degrees = trans)   181.19
! DIHEdral  H11  C1   C10  C19 ! flexible dihedral ???   -58.28
! DIHEdral  H12  C1   C10  C5  ! flat ? (180 degrees = trans)   180.75
! DIHEdral  H12  C1   C10  C9  ! flexible dihedral ???   -59.71
! DIHEdral  H12  C1   C10  C19 ! flexible dihedral ???    60.82
! DIHEdral  C2   C1   C10  C5  ! flexible dihedral ???   -58.81
! DIHEdral  C2   C1   C10  C9  ! flexible dihedral ???    60.73
! DIHEdral  C2   C1   C10  C19 ! flat ? (180 degrees = trans)   181.26
! DIHEdral  C1   C2   C3   H3  ! flexible dihedral ???    60.48
! DIHEdral  C1   C2   C3   C4  ! flexible dihedral ???   -59.11
! DIHEdral  C1   C2   C3   O1  ! flat ? (180 degrees = trans)   180.48
! DIHEdral  H21  C2   C3   H3  ! flat ? (180 degrees = trans)   177.15
! DIHEdral  H21  C2   C3   C4  ! flexible dihedral ???    57.56
! DIHEdral  H21  C2   C3   O1  ! flexible dihedral ???   -62.85
! DIHEdral  H22  C2   C3   H3  ! flexible dihedral ???   -56.17
! DIHEdral  H22  C2   C3   C4  ! flat ? (180 degrees = trans)   184.24
! DIHEdral  H22  C2   C3   O1  ! flexible dihedral ???    63.83
! DIHEdral  C2   C3   C4   H41 ! flexible dihedral ???   -60.08
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! DIHEdral  C2   C3   C4   H42 ! flat ? (180 degrees = trans)   179.96
! DIHEdral  C2   C3   C4   C5  ! flexible dihedral ???    59.93
! DIHEdral  H3   C3   C4   H41 ! flat ? (180 degrees = trans)   180.00
! DIHEdral  H3   C3   C4   H42 ! flexible dihedral ???    60.04
! DIHEdral  H3   C3   C4   C5  ! flexible dihedral ???   -59.99
! DIHEdral  O1   C3   C4   H41 ! flexible dihedral ???    60.26
! DIHEdral  O1   C3   C4   H42 ! flexible dihedral ???   -59.70
! DIHEdral  O1   C3   C4   C5  ! flat ? (180 degrees = trans)   180.27
! DIHEdral  C2   C3   O1   H1  ! flexible dihedral ???   -50.93
! DIHEdral  H3   C3   O1   H1  ! flexible dihedral ???    69.22
! DIHEdral  C4   C3   O1   H1  ! flat ? (180 degrees = trans)   188.77
! DIHEdral  C3   C4   C5   H5  ! flexible dihedral ???    57.98
! DIHEdral  C3   C4   C5   C6  ! flat ? (180 degrees = trans)   177.97
! DIHEdral  C3   C4   C5   C10 ! flexible dihedral ???   -57.95
! DIHEdral  H41  C4   C5   H5  ! flat ? (180 degrees = trans)   178.78
! DIHEdral  H41  C4   C5   C6  ! flexible dihedral ???   -61.23
! DIHEdral  H41  C4   C5   C10 ! flexible dihedral ???    62.86
! DIHEdral  H42  C4   C5   H5  ! flexible dihedral ???   -62.82
! DIHEdral  H42  C4   C5   C6  ! flexible dihedral ???    57.16
! DIHEdral  H42  C4   C5   C10 ! flat ? (180 degrees = trans)   181.25
! DIHEdral  C4   C5   C6   H61 ! flexible dihedral ???   -54.20
! DIHEdral  C4   C5   C6   H62 ! flat ? (180 degrees = trans)   185.79
! DIHEdral  C4   C5   C6   C7  ! flexible dihedral ???    65.79
! DIHEdral  H5   C5   C6   H61 ! flexible dihedral ???    69.97
! DIHEdral  H5   C5   C6   H62 ! flexible dihedral ???   -50.04
! DIHEdral  H5   C5   C6   C7  ! flat ? (180 degrees = trans)   189.95
! DIHEdral  C10  C5   C6   H61 ! flat ? (180 degrees = trans)   181.66
! DIHEdral  C10  C5   C6   H62 ! flexible dihedral ???    61.65
! DIHEdral  C10  C5   C6   C7  ! flexible dihedral ???   -58.36
! DIHEdral  C4   C5   C10  C1  ! flexible dihedral ???    54.29
! DIHEdral  C4   C5   C10  C9  ! flexible dihedral ???   -67.83
! DIHEdral  C4   C5   C10  C19 ! flat ? (180 degrees = trans)   172.83
! DIHEdral  H5   C5   C10  C1  ! flexible dihedral ???   -67.25
! DIHEdral  H5   C5   C10  C9  ! flat ? (180 degrees = trans)   170.64
! DIHEdral  H5   C5   C10  C19 ! flexible dihedral ???    51.30
! DIHEdral  C6   C5   C10  C1  ! flat ? (180 degrees = trans)   179.95
! DIHEdral  C6   C5   C10  C9  ! flexible dihedral ???    57.83
! DIHEdral  C6   C5   C10  C19 ! flexible dihedral ???   -61.51
! DIHEdral  C5   C6   C7   H71 ! flexible dihedral ???   -60.18
! DIHEdral  C5   C6   C7   H72 ! flat ? (180 degrees = trans)   179.83
! DIHEdral  C5   C6   C7   C8  ! flexible dihedral ???    59.83
! DIHEdral  H61  C6   C7   H71 ! flexible dihedral ???    61.35
! DIHEdral  H61  C6   C7   H72 ! flexible dihedral ???   -58.64
! DIHEdral  H61  C6   C7   C8  ! flat ? (180 degrees = trans)   181.36
! DIHEdral  H62  C6   C7   H71 ! flat ? (180 degrees = trans)   178.27
! DIHEdral  H62  C6   C7   H72 ! flexible dihedral ???    58.28
! DIHEdral  H62  C6   C7   C8  ! flexible dihedral ???   -61.72
! DIHEdral  C6   C7   C8   H8  ! flexible dihedral ???    60.70
! DIHEdral  C6   C7   C8   C9  ! flexible dihedral ???   -59.29
! DIHEdral  C6   C7   C8   C14 ! flat ? (180 degrees = trans)   180.70
! DIHEdral  H71  C7   C8   H8  ! flat ? (180 degrees = trans)   183.70
! DIHEdral  H71  C7   C8   C9  ! flexible dihedral ???    63.70
! DIHEdral  H71  C7   C8   C14 ! flexible dihedral ???   -56.30
! DIHEdral  H72  C7   C8   H8  ! flexible dihedral ???   -62.28
! DIHEdral  H72  C7   C8   C9  ! flat ? (180 degrees = trans)   177.72
! DIHEdral  H72  C7   C8   C14 ! flexible dihedral ???    57.72
! DIHEdral  C7   C8   C9   H9  ! flexible dihedral ???   -60.83
! DIHEdral  C7   C8   C9   C10 ! flexible dihedral ???    59.17
! DIHEdral  C7   C8   C9   C11 ! flat ? (180 degrees = trans)   181.00
! DIHEdral  H8   C8   C9   H9  ! flat ? (180 degrees = trans)   181.80
! DIHEdral  H8   C8   C9   C10 ! flexible dihedral ???   -58.20
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! DIHEdral  H8   C8   C9   C11 ! flexible dihedral ???    63.62
! DIHEdral  C14  C8   C9   H9  ! flexible dihedral ???    61.20
! DIHEdral  C14  C8   C9   C10 ! flat ? (180 degrees = trans)   181.20
! DIHEdral  C14  C8   C9   C11 ! flexible dihedral ???   -56.98
! DIHEdral  C7   C8   C14  C13 ! flat ? (180 degrees = trans)   179.12
! DIHEdral  C7   C8   C14  H14 ! flexible dihedral ???    59.10
! DIHEdral  C7   C8   C14  C15 ! flexible dihedral ???   -59.80
! DIHEdral  H8   C8   C14  C13 ! flexible dihedral ???   -61.90
! DIHEdral  H8   C8   C14  H14 ! flat ? (180 degrees = trans)   178.08
! DIHEdral  H8   C8   C14  C15 ! flexible dihedral ???    59.18
! DIHEdral  C9   C8   C14  C13 ! flexible dihedral ???    60.12
! DIHEdral  C9   C8   C14  H14 ! flexible dihedral ???   -59.90
! DIHEdral  C9   C8   C14  C15 ! flat ? (180 degrees = trans)   181.20
! DIHEdral  C8   C9   C10  C1  ! flat ? (180 degrees = trans)   181.41
! DIHEdral  C8   C9   C10  C5  ! flexible dihedral ???   -59.37
! DIHEdral  C8   C9   C10  C19 ! flexible dihedral ???    61.09
! DIHEdral  H9   C9   C10  C1  ! flexible dihedral ???   -57.43
! DIHEdral  H9   C9   C10  C5  ! flexible dihedral ???    61.80
! DIHEdral  H9   C9   C10  C19 ! flat ? (180 degrees = trans)   182.26
! DIHEdral  C11  C9   C10  C1  ! flexible dihedral ???    60.90
! DIHEdral  C11  C9   C10  C5  ! flat ? (180 degrees = trans)   180.13
! DIHEdral  C11  C9   C10  C19 ! flexible dihedral ???   -59.41
! DIHEdral  C8   C9   C11 H111 ! flexible dihedral ???   -61.63
! DIHEdral  C8   C9   C11 H112 ! flat ? (180 degrees = trans)   178.40
! DIHEdral  C8   C9   C11  C12 ! flexible dihedral ???    58.41
! DIHEdral  H9   C9   C11 H111 ! flat ? (180 degrees = trans)   178.61
! DIHEdral  H9   C9   C11 H112 ! flexible dihedral ???    58.64
! DIHEdral  H9   C9   C11  C12 ! flexible dihedral ???   -61.36
! DIHEdral  C10  C9   C11 H111 ! flexible dihedral ???    59.94
! DIHEdral  C10  C9   C11 H112 ! flexible dihedral ???   -60.03
! DIHEdral  C10  C9   C11  C12 ! flat ? (180 degrees = trans)   179.97
! DIHEdral  C1   C10  C19 H191 ! flat ? (0 degrees = cis)     0.00
! DIHEdral  C5   C10  C19 H192 ! flat ? (0 degrees = cis)     1.84
! DIHEdral  C9   C10  C19 H193 ! flat ? (0 degrees = cis)     2.78
! DIHEdral  C9   C11  C12 H121 ! flat ? (180 degrees = trans)   179.49
! DIHEdral  C9   C11  C12  C13 ! flexible dihedral ???   -60.79
! DIHEdral  C9   C11  C12  O2  ! flexible dihedral ???    59.49
! DIHEdral H111  C11  C12 H121 ! flexible dihedral ???   -58.55
! DIHEdral H111  C11  C12  C13 ! flexible dihedral ???    61.16
! DIHEdral H111  C11  C12  O2  ! flat ? (180 degrees = trans)   181.45
! DIHEdral H112  C11  C12 H121 ! flexible dihedral ???    57.55
! DIHEdral H112  C11  C12  C13 ! flat ? (180 degrees = trans)   177.27
! DIHEdral H112  C11  C12  O2  ! flexible dihedral ???   -62.45
! DIHEdral  C11  C12  C13  C14 ! flexible dihedral ???    57.69
! DIHEdral  C11  C12  C13  C18 ! flexible dihedral ???   -60.01
! DIHEdral H121  C12  C13  C14 ! flat ? (180 degrees = trans)   178.36
! DIHEdral H121  C12  C13  C18 ! flexible dihedral ???    60.66
! DIHEdral  O2   C12  C13  C14 ! flexible dihedral ???   -63.27
! DIHEdral  O2   C12  C13  C18 ! flat ? (180 degrees = trans)   179.03
! DIHEdral  C12  C13  C14  C8  ! flexible dihedral ???   -59.72
! DIHEdral  C12  C13  C14  H14 ! flexible dihedral ???    60.64
! DIHEdral  C12  C13  C14  C15 ! flat ? (180 degrees = trans)   172.08
! DIHEdral  C17  C13  C14  C8  ! flat ? (180 degrees = trans)   177.13
! DIHEdral  C17  C13  C14  H14 ! flexible dihedral ???   -62.51
! DIHEdral  C18  C13  C14  C8  ! flexible dihedral ???    59.76
! DIHEdral  C18  C13  C14  H14 ! flat ? (180 degrees = trans)   180.12
! DIHEdral  C18  C13  C14  C15 ! flexible dihedral ???   -68.44
! DIHEdral  C14  C13  C17  C20 ! flat ? (180 degrees = trans)   189.18
! DIHEdral  C18  C13  C17  C16 ! flexible dihedral ???    69.81
! DIHEdral  C18  C13  C17  H17 ! flat ? (180 degrees = trans)   189.82
! DIHEdral  C18  C13  C17  C20 ! flexible dihedral ???   -56.80
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! DIHEdral  C12  C13  C18 H181 ! flat ? (0 degrees = cis)     0.00
! DIHEdral  C14  C13  C18 H182 ! flat ? (0 degrees = cis)     3.74
! DIHEdral  C13  C14  C15 H152 ! flexible dihedral ???    86.33
! DIHEdral  C14  C15  C16  C17 ! flat ? (0 degrees = cis)     5.80
! DIHEdral H151  C15  C16 H161 ! flat ? (0 degrees = cis)     5.25
! DIHEdral H152  C15  C16 H162 ! flat ? (0 degrees = cis)     6.32
! DIHEdral  C15  C16  C17  H17 ! flexible dihedral ???   -94.45
! DIHEdral H161  C16  C17  C20 ! flexible dihedral ???   -89.61
! DIHEdral H162  C16  C17  C13 ! flexible dihedral ???   -91.38
! DIHEdral  C13  C17  C20  H20 ! flexible dihedral ???    66.67
! DIHEdral  C13  C17  C20  C21 ! flexible dihedral ???   -53.35
! DIHEdral  C13  C17  C20  C22 ! flat ? (180 degrees = trans)   180.53
! DIHEdral  C16  C17  C20  H20 ! flexible dihedral ???   -54.79
! DIHEdral  C16  C17  C20  C21 ! flat ? (180 degrees = trans)   185.19
! DIHEdral  C16  C17  C20  C22 ! flexible dihedral ???    59.07
! DIHEdral  H17  C17  C20  H20 ! flat ? (180 degrees = trans)   186.35
! DIHEdral  H17  C17  C20  C21 ! flexible dihedral ???    66.33
! DIHEdral  H17  C17  C20  C22 ! flexible dihedral ???   -59.79
! DIHEdral  C17  C20  C21 H211 ! flat ? (0 degrees = cis)     0.00
! DIHEdral  H20  C20  C21 H212 ! flat ? (0 degrees = cis)    -0.64
! DIHEdral  C22  C20  C21 H213 ! flat ? (0 degrees = cis)     6.45
! DIHEdral  C17  C20  C22 H221 ! flexible dihedral ???   -52.16
! DIHEdral  C17  C20  C22 H222 ! flat ? (180 degrees = trans)   187.88
! DIHEdral  C17  C20  C22  C23 ! flexible dihedral ???    67.87
! DIHEdral  H20  C20  C22 H221 ! flexible dihedral ???    62.67
! DIHEdral  H20  C20  C22 H222 ! flexible dihedral ???   -57.30
! DIHEdral  H20  C20  C22  C23 ! flat ? (180 degrees = trans)   182.70
! DIHEdral  C21  C20  C22 H221 ! flat ? (180 degrees = trans)   175.79
! DIHEdral  C21  C20  C22 H222 ! flexible dihedral ???    55.82
! DIHEdral  C21  C20  C22  C23 ! flexible dihedral ???   -64.18
! DIHEdral  C20  C22  C23 H231 ! flexible dihedral ???    51.62
! DIHEdral  C20  C22  C23 H232 ! flexible dihedral ???   -68.36
! DIHEdral  C20  C22  C23  C24 ! flat ? (180 degrees = trans)   171.63
! DIHEdral H221  C22  C23 H231 ! flat ? (180 degrees = trans)   172.08
! DIHEdral H221  C22  C23 H232 ! flexible dihedral ???    52.10
! DIHEdral H221  C22  C23  C24 ! flexible dihedral ???   -67.91
! DIHEdral H222  C22  C23 H231 ! flexible dihedral ???   -68.83
! DIHEdral H222  C22  C23 H232 ! flat ? (180 degrees = trans)   171.19
! DIHEdral H222  C22  C23  C24 ! flexible dihedral ???    51.18
! DIHEdral  C22  C23  C24  O3  ! flat ? (0 degrees = cis)    -8.50
! DIHEdral  C22  C23  C24  O4  ! flat ? (180 degrees = trans)   171.64
! DIHEdral H231  C23  C24  O4  ! flexible dihedral ???   -64.92

 { edit these IMPRopers if necessary }
 IMPRoper  C1   H11  H12  C2  ! chirality or flatness improper    41.49
 IMPRoper  C1   C2   C3   O1  ! dihedral improper                180.48
 IMPRoper  C2   C1   H21  H22 ! chirality or flatness improper    33.57
 IMPRoper  C3   C2   H3   C4  ! chirality or flatness improper    37.92
 IMPRoper  C3   C4   C5   C6  ! dihedral improper                177.97
 IMPRoper  C4   C3   H41  H42 ! chirality or flatness improper    33.25
 IMPRoper  C5   C4   H5   C6  ! chirality or flatness improper   -37.38
 IMPRoper  C6   C5   H61  H62 ! chirality or flatness improper    33.12
 IMPRoper  C7   C6   H71  H72 ! chirality or flatness improper    32.97
 IMPRoper  C8   C7   H8   C9  ! chirality or flatness improper    38.50
 IMPRoper  C9   C8   H9   C10 ! chirality or flatness improper   -38.36
 IMPRoper  C10  C1   C5   C9  ! chirality or flatness improper   -34.83
 IMPRoper  C11  C9  H111 H112 ! chirality or flatness improper    33.05
 IMPRoper  C12  C11 H121  C13 ! chirality or flatness improper   -38.06
 IMPRoper  C13  C12  C14  C17 ! chirality or flatness improper   -36.07
! IMPRoper  C13  C17  C20  H20 ! dihedral improper                 66.67
! IMPRoper  C13  C17  C20  C21 ! dihedral improper                -53.35
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 IMPRoper  C14  C8   C13  H14 ! chirality or flatness improper    31.42
 IMPRoper  C15  C14 H151 H152 ! chirality or flatness improper    33.07
 IMPRoper  C16  C15 H161 H162 ! chirality or flatness improper    33.47
 IMPRoper  C17  C13  C16  H17 ! chirality or flatness improper   -28.84
 IMPRoper  C18  C13 H181 H182 ! chirality or flatness improper   -33.05
 IMPRoper  C19  C10 H191 H192 ! chirality or flatness improper   -33.22
 IMPRoper  C20  C17  H20  C21 ! chirality or flatness improper    33.61
 IMPRoper  C21  C20 H211 H212 ! chirality or flatness improper   -33.49
 IMPRoper  C22  C20 H221 H222 ! chirality or flatness improper    33.34
 IMPRoper  C23  C22 H231 H232 ! chirality or flatness improper    33.06
 IMPRoper  C24  C23  O3   O4  ! chirality or flatness improper     0.08

 { edit any DONOrs and ACCEptors if necessary }
 ACCEptor  O1   C3
 ACCEptor  O2   C12
 ACCEptor  O3   C24
 ACCEptor  O4   C24

END { RESIdue DHO }



PC2_top.txt
Remarks ../../tmp/hicup_btcpxq_9457/PC2_top.txt
Remarks Created by XPLO2D V. 001221/2.8.9 at Mon Apr 23 13:31:21 2001 for
A. Nonymous
Remarks Auto-generated by XPLO2D from file ../../tmp/hicup_btcpxq_
9457/user.pdb
Remarks You *MUST* check/edit MASSes and CHARges !!!
Remarks Check DONOrs and ACCEptors
Remarks Verify IMPROpers yourself
Remarks DIHEdrals which are not flat are commented out

 set echo=false end

 { edit masses if necessary }
 MASS CX1    12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX2     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX3     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX4    12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX5     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX6    12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX7     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX8     1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX9    12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX10    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX11    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX12   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX13    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX14    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX15   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX16    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX17    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX18    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX19   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX20    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX21    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX22    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX23   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX24    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX25    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
```

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MASS HX26    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX27   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS CX28   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX29    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX30    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX31   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX32    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX33    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX34   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX35    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX36    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX37   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX38    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX39    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX40   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX41    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX42    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX43   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX44    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX45    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX46   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX47    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX48    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX49   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX50    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX51    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX52   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX53    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX54    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX55   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX56    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX57    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX58   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX59    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX60    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX61   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX62    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX63    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX64   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX65    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX66    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX67   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX68    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX69    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX70   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX71    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX72    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX73   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX74    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX75    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX76   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX77    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX78    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX79    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX80   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS CX81   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX82    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX83    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS CX84   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
MASS HX85    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
MASS HX86    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
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 MASS CX87   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX88    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX89    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX90   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX91    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX92    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX93   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX94    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX95    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX96   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX97    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX98    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX99   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX1A    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX1B    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX10   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX1C    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX1D    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX1A   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX1E    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX1F    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX1B   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX1G    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX1H    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX11   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX1I    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX1J    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX1C   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX1K    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX1L    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX1D   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX1M    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX1N    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX1E   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX12    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX1O    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX1F   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX1P    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX1Q    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX1G   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX1R    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX1S    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS CX1H   12.01100 ! assuming C -> 12.01100 + 1.008 * 0 (Hs)
 MASS HX1T    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX1U    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS HX1V    1.00800 ! assuming H -> 1.00800 + 1.008 * 0 (Hs)
 MASS NX13   14.00700 ! assuming N -> 14.00700 + 1.008 * 0 (Hs)
 MASS OX13   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
 MASS OX1A   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
 MASS OX1B   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
 MASS OX1C   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
 MASS OX1D   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
 MASS OX1E   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
 MASS OX14   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
 MASS OX1F   15.99900 ! assuming O -> 15.99900 + 1.008 * 0 (Hs)
 MASS PX14   30.97400 ! assuming P -> 30.97400 + 1.008 * 0 (Hs)

 autogenerate angles=true end

RESIdue PC2
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GROUp
 ATOM  C1   TYPE CX1   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H11  TYPE HX2   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H12  TYPE HX3   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C2   TYPE CX4   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H2   TYPE HX5   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C3   TYPE CX6   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H31  TYPE HX7   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H32  TYPE HX8   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C4   TYPE CX9   CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H41  TYPE HX10  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H42  TYPE HX11  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C5   TYPE CX12  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H51  TYPE HX13  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H52  TYPE HX14  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C6   TYPE CX15  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H61  TYPE HX16  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H62  TYPE HX17  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H63  TYPE HX18  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C7   TYPE CX19  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H71  TYPE HX20  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H72  TYPE HX21  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H73  TYPE HX22  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C8   TYPE CX23  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H81  TYPE HX24  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H82  TYPE HX25  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  H83  TYPE HX26  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C11  TYPE CX27  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C12  TYPE CX28  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H121  TYPE HX29  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H122  TYPE HX30  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C13  TYPE CX31  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H131  TYPE HX32  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H132  TYPE HX33  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C14  TYPE CX34  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H141  TYPE HX35  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H142  TYPE HX36  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C15  TYPE CX37  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H151  TYPE HX38  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H152  TYPE HX39  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C16  TYPE CX40  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H161  TYPE HX41  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H162  TYPE HX42  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C17  TYPE CX43  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H171  TYPE HX44  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H172  TYPE HX45  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C18  TYPE CX46  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H181  TYPE HX47  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H182  TYPE HX48  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C19  TYPE CX49  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H191  TYPE HX50  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H192  TYPE HX51  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C20  TYPE CX52  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H201  TYPE HX53  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H202  TYPE HX54  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C21  TYPE CX55  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H211  TYPE HX56  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H212  TYPE HX57  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C22  TYPE CX58  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H221  TYPE HX59  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H222  TYPE HX60  CHARge  0.0  END ! Nr of Hs =  0
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ATOM  C23  TYPE CX61  CHARge  0.0  END ! Nr of Hs =  0
ATOM H231  TYPE HX62  CHARge  0.0  END ! Nr of Hs =  0
ATOM H232  TYPE HX63  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C24  TYPE CX64  CHARge  0.0  END ! Nr of Hs =  0
ATOM H241  TYPE HX65  CHARge  0.0  END ! Nr of Hs =  0
ATOM H242  TYPE HX66  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C25  TYPE CX67  CHARge  0.0  END ! Nr of Hs =  0
ATOM H251  TYPE HX68  CHARge  0.0  END ! Nr of Hs =  0
ATOM H252  TYPE HX69  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C26  TYPE CX70  CHARge  0.0  END ! Nr of Hs =  0
ATOM H261  TYPE HX71  CHARge  0.0  END ! Nr of Hs =  0
ATOM H262  TYPE HX72  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C27  TYPE CX73  CHARge  0.0  END ! Nr of Hs =  0
ATOM H271  TYPE HX74  CHARge  0.0  END ! Nr of Hs =  0
ATOM H272  TYPE HX75  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C28  TYPE CX76  CHARge  0.0  END ! Nr of Hs =  0
ATOM H281  TYPE HX77  CHARge  0.0  END ! Nr of Hs =  0
ATOM H282  TYPE HX78  CHARge  0.0  END ! Nr of Hs =  0
ATOM H283  TYPE HX79  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C31  TYPE CX80  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C32  TYPE CX81  CHARge  0.0  END ! Nr of Hs =  0
ATOM H321  TYPE HX82  CHARge  0.0  END ! Nr of Hs =  0
ATOM H322  TYPE HX83  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C33  TYPE CX84  CHARge  0.0  END ! Nr of Hs =  0
ATOM H331  TYPE HX85  CHARge  0.0  END ! Nr of Hs =  0
ATOM H332  TYPE HX86  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C34  TYPE CX87  CHARge  0.0  END ! Nr of Hs =  0
ATOM H341  TYPE HX88  CHARge  0.0  END ! Nr of Hs =  0
ATOM H342  TYPE HX89  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C35  TYPE CX90  CHARge  0.0  END ! Nr of Hs =  0
ATOM H351  TYPE HX91  CHARge  0.0  END ! Nr of Hs =  0
ATOM H352  TYPE HX92  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C36  TYPE CX93  CHARge  0.0  END ! Nr of Hs =  0
ATOM H361  TYPE HX94  CHARge  0.0  END ! Nr of Hs =  0
ATOM H362  TYPE HX95  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C37  TYPE CX96  CHARge  0.0  END ! Nr of Hs =  0
ATOM H371  TYPE HX97  CHARge  0.0  END ! Nr of Hs =  0
ATOM H372  TYPE HX98  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C38  TYPE CX99  CHARge  0.0  END ! Nr of Hs =  0
ATOM H381  TYPE HX1A  CHARge  0.0  END ! Nr of Hs =  0
ATOM H382  TYPE HX1B  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C39  TYPE CX10  CHARge  0.0  END ! Nr of Hs =  0
ATOM H391  TYPE HX1C  CHARge  0.0  END ! Nr of Hs =  0
ATOM H392  TYPE HX1D  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C40  TYPE CX1A  CHARge  0.0  END ! Nr of Hs =  0
ATOM H401  TYPE HX1E  CHARge  0.0  END ! Nr of Hs =  0
ATOM H402  TYPE HX1F  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C41  TYPE CX1B  CHARge  0.0  END ! Nr of Hs =  0
ATOM H411  TYPE HX1G  CHARge  0.0  END ! Nr of Hs =  0
ATOM H412  TYPE HX1H  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C42  TYPE CX11  CHARge  0.0  END ! Nr of Hs =  0
ATOM H421  TYPE HX1I  CHARge  0.0  END ! Nr of Hs =  0
ATOM H422  TYPE HX1J  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C43  TYPE CX1C  CHARge  0.0  END ! Nr of Hs =  0
ATOM H431  TYPE HX1K  CHARge  0.0  END ! Nr of Hs =  0
ATOM H432  TYPE HX1L  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C44  TYPE CX1D  CHARge  0.0  END ! Nr of Hs =  0
ATOM H441  TYPE HX1M  CHARge  0.0  END ! Nr of Hs =  0
ATOM H442  TYPE HX1N  CHARge  0.0  END ! Nr of Hs =  0
ATOM  C45  TYPE CX1E  CHARge  0.0  END ! Nr of Hs =  0
ATOM H451  TYPE HX12  CHARge  0.0  END ! Nr of Hs =  0
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 ATOM H452  TYPE HX1O  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C46  TYPE CX1F  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H461  TYPE HX1P  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H462  TYPE HX1Q  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C47  TYPE CX1G  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H471  TYPE HX1R  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H472  TYPE HX1S  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  C48  TYPE CX1H  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H481  TYPE HX1T  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H482  TYPE HX1U  CHARge  0.0  END ! Nr of Hs =  0
 ATOM H483  TYPE HX1V  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  N    TYPE NX13  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  O2   TYPE OX13  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  O3   TYPE OX1A  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  O11  TYPE OX1B  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  O31  TYPE OX1C  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  O1P  TYPE OX1D  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  O2P  TYPE OX1E  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  O3P  TYPE OX14  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  O4P  TYPE OX1F  CHARge  0.0  END ! Nr of Hs =  0
 ATOM  P    TYPE PX14  CHARge  0.0  END ! Nr of Hs =  0

 BOND  C1   H11      BOND  C1   H12      BOND  C1   C2       BOND  C1   O3P
 BOND  C2   H2       BOND  C2   C3       BOND  C2   O2       BOND  C3   H31
 BOND  C3   H32      BOND  C3   O3       BOND  C4   H41      BOND  C4   H42
 BOND  C4   C5       BOND  C4   O4P      BOND  C5   H51      BOND  C5   H52
 BOND  C5   N        BOND  C6   H61      BOND  C6   H62      BOND  C6   H63
 BOND  C6   N        BOND  C7   H71      BOND  C7   H72      BOND  C7   H73
 BOND  C7   N        BOND  C8   H81      BOND  C8   H82      BOND  C8   H83
 BOND  C8   N        BOND  C11  C12      BOND  C11  O3       BOND  C11  O11
 BOND  C12 H121      BOND  C12 H122      BOND  C12  C13      BOND  C13 H131
 BOND  C13 H132      BOND  C13  C14      BOND  C14 H141      BOND  C14 H142
 BOND  C14  C15      BOND  C15 H151      BOND  C15 H152      BOND  C15  C16
 BOND  C16 H161      BOND  C16 H162      BOND  C16  C17      BOND  C17 H171
 BOND  C17 H172      BOND  C17  C18      BOND  C18 H181      BOND  C18 H182
 BOND  C18  C19      BOND  C19 H191      BOND  C19 H192      BOND  C19  C20
 BOND  C20 H201      BOND  C20 H202      BOND  C20  C21      BOND  C21 H211
 BOND  C21 H212      BOND  C21  C22      BOND  C22 H221      BOND  C22 H222
 BOND  C22  C23      BOND  C23 H231      BOND  C23 H232      BOND  C23  C24
 BOND  C24 H241      BOND  C24 H242      BOND  C24  C25      BOND  C25 H251
 BOND  C25 H252      BOND  C25  C26      BOND  C26 H261      BOND  C26 H262
 BOND  C26  C27      BOND  C27 H271      BOND  C27 H272      BOND  C27  C28
 BOND  C28 H281      BOND  C28 H282      BOND  C28 H283      BOND  C31  C32
 BOND  C31  O2       BOND  C31  O31      BOND  C32 H321      BOND  C32 H322
 BOND  C32  C33      BOND  C33 H331      BOND  C33 H332      BOND  C33  C34
 BOND  C34 H341      BOND  C34 H342      BOND  C34  C35      BOND  C35 H351
 BOND  C35 H352      BOND  C35  C36      BOND  C36 H361      BOND  C36 H362
 BOND  C36  C37      BOND  C37 H371      BOND  C37 H372      BOND  C37  C38
 BOND  C38 H381      BOND  C38 H382      BOND  C38  C39      BOND  C39 H391
 BOND  C39 H392      BOND  C39  C40      BOND  C40 H401      BOND  C40 H402
 BOND  C40  C41      BOND  C41 H411      BOND  C41 H412      BOND  C41  C42
 BOND  C42 H421      BOND  C42 H422      BOND  C42  C43      BOND  C43 H431
 BOND  C43 H432      BOND  C43  C44      BOND  C44 H441      BOND  C44 H442
 BOND  C44  C45      BOND  C45 H451      BOND  C45 H452      BOND  C45  C46
 BOND  C46 H461      BOND  C46 H462      BOND  C46  C47      BOND  C47 H471
 BOND  C47 H472      BOND  C47  C48      BOND  C48 H481      BOND  C48 H482
 BOND  C48 H483      BOND  O1P  P        BOND  O2P  P        BOND  O3P  P
 BOND  O4P  P

  { edit these DIHEdrals if necessary }
! DIHEdral  H11  C1   C2   O2  ! flexible dihedral ???    86.47
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! DIHEdral  H11  C1   O3P  P   ! flexible dihedral ???   -69.40
! DIHEdral  H12  C1   O3P  P   ! flexible dihedral ???    59.35
! DIHEdral  C2   C1   O3P  P   ! flat ? (180 degrees = trans)   174.98
! DIHEdral  C1   C2   C3   H32 ! flexible dihedral ???    89.50
! DIHEdral  H2   C2   C3   H31 ! flexible dihedral ???    93.69
! DIHEdral  O2   C2   C3   O3  ! flexible dihedral ???    81.45
! DIHEdral  C2   C3   O3   C11 ! flat ? (180 degrees = trans)   179.15
! DIHEdral  H31  C3   O3   C11 ! flexible dihedral ???   -59.60
! DIHEdral  H32  C3   O3   C11 ! flexible dihedral ???    57.89
! DIHEdral  H41  C4   C5   H51 ! flexible dihedral ???   -97.33
! DIHEdral  H42  C4   C5   N   ! flexible dihedral ???   -97.31
! DIHEdral  O4P  C4   C5   H52 ! flexible dihedral ???   -97.29
! DIHEdral  H41  C4   O4P  P   ! flexible dihedral ???   -53.67
! DIHEdral  C4   C5   N    C6  ! flexible dihedral ???   -62.17
! DIHEdral  C4   C5   N    C7  ! flexible dihedral ???    60.35
! DIHEdral  C4   C5   N    C8  ! flat ? (180 degrees = trans)   179.65
! DIHEdral  H51  C5   N    C6  ! flexible dihedral ???    58.15
! DIHEdral  H51  C5   N    C7  ! flat ? (180 degrees = trans)   180.67
! DIHEdral  H51  C5   N    C8  ! flexible dihedral ???   -60.03
! DIHEdral  H52  C5   N    C6  ! flat ? (180 degrees = trans)   177.50
! DIHEdral  H52  C5   N    C7  ! flexible dihedral ???   -59.98
! DIHEdral  H52  C5   N    C8  ! flexible dihedral ???    59.32
! DIHEdral  H61  C6   N    C5  ! flat ? (180 degrees = trans)   180.00
! DIHEdral  H61  C6   N    C7  ! flexible dihedral ???    55.92
! DIHEdral  H61  C6   N    C8  ! flexible dihedral ???   -61.55
! DIHEdral  H62  C6   N    C5  ! flexible dihedral ???   -59.98
! DIHEdral  H62  C6   N    C7  ! flat ? (180 degrees = trans)   175.94
! DIHEdral  H62  C6   N    C8  ! flexible dihedral ???    58.47
! DIHEdral  H63  C6   N    C5  ! flexible dihedral ???    60.00
! DIHEdral  H63  C6   N    C7  ! flexible dihedral ???   -64.09
! DIHEdral  H63  C6   N    C8  ! flat ? (180 degrees = trans)   178.45
! DIHEdral  H71  C7   N    C5  ! flat ? (180 degrees = trans)   179.99
! DIHEdral  H71  C7   N    C6  ! flexible dihedral ???   -57.04
! DIHEdral  H71  C7   N    C8  ! flexible dihedral ???    60.42
! DIHEdral  H72  C7   N    C5  ! flexible dihedral ???   -60.00
! DIHEdral  H72  C7   N    C6  ! flexible dihedral ???    62.96
! DIHEdral  H72  C7   N    C8  ! flat ? (180 degrees = trans)   180.42
! DIHEdral  H73  C7   N    C5  ! flexible dihedral ???    60.02
! DIHEdral  H73  C7   N    C6  ! flat ? (180 degrees = trans)   182.98
! DIHEdral  H73  C7   N    C8  ! flexible dihedral ???   -59.56
! DIHEdral  H81  C8   N    C5  ! flat ? (180 degrees = trans)   179.98
! DIHEdral  H81  C8   N    C6  ! flexible dihedral ???    60.34
! DIHEdral  H81  C8   N    C7  ! flexible dihedral ???   -58.10
! DIHEdral  H82  C8   N    C5  ! flexible dihedral ???   -59.99
! DIHEdral  H82  C8   N    C6  ! flat ? (180 degrees = trans)   180.38
! DIHEdral  H82  C8   N    C7  ! flexible dihedral ???    61.94
! DIHEdral  H83  C8   N    C5  ! flexible dihedral ???    60.02
! DIHEdral  H83  C8   N    C6  ! flexible dihedral ???   -59.61
! DIHEdral  H83  C8   N    C7  ! flat ? (180 degrees = trans)   181.95
! DIHEdral  O3   C11  C12 H122 ! flexible dihedral ???    89.54
! DIHEdral  O11  C11  C12 H122 ! flexible dihedral ???   -88.76
! DIHEdral  C11  C12  C13  C14 ! flexible dihedral ???   -87.15
! DIHEdral H121  C12  C13 H131 ! flexible dihedral ???   -83.14
! DIHEdral H122  C12  C13 H132 ! flexible dihedral ???   -91.20
! DIHEdral  C12  C13  C14 H141 ! flexible dihedral ???    97.07
! DIHEdral H132  C13  C14  C15 ! flexible dihedral ???    92.41
! DIHEdral H151  C15  C16  C17 ! flexible dihedral ???   -97.50
! DIHEdral  C16  C17  C18  C19 ! flexible dihedral ???    83.54
! DIHEdral H171  C17  C18 H181 ! flexible dihedral ???    83.88
! DIHEdral H172  C17  C18 H182 ! flexible dihedral ???    83.18
! DIHEdral  C17  C18  C19 H191 ! flexible dihedral ???    62.68
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! DIHEdral  C17  C18  C19 H192 ! flexible dihedral ???   -57.30
! DIHEdral  C17  C18  C19  C20 ! flat ? (180 degrees = trans)   182.66
! DIHEdral H181  C18  C19 H191 ! flat ? (180 degrees = trans)   182.72
! DIHEdral H181  C18  C19 H192 ! flexible dihedral ???    62.73
! DIHEdral H181  C18  C19  C20 ! flexible dihedral ???   -57.30
! DIHEdral H182  C18  C19 H191 ! flexible dihedral ???   -57.37
! DIHEdral H182  C18  C19 H192 ! flat ? (180 degrees = trans)   182.64
! DIHEdral H182  C18  C19  C20 ! flexible dihedral ???    62.61
! DIHEdral  C18  C19  C20  C21 ! flat ? (0 degrees = cis)    -0.03
! DIHEdral H191  C19  C20 H201 ! flat ? (0 degrees = cis)     0.43
! DIHEdral H192  C19  C20 H202 ! flat ? (0 degrees = cis)    -0.51
! DIHEdral  C20  C21  C22 H221 ! flexible dihedral ???   -64.97
! DIHEdral  C20  C21  C22 H222 ! flat ? (180 degrees = trans)   175.02
! DIHEdral  C20  C21  C22  C23 ! flexible dihedral ???    55.02
! DIHEdral H211  C21  C22 H221 ! flexible dihedral ???    57.48
! DIHEdral H211  C21  C22 H222 ! flexible dihedral ???   -62.53
! DIHEdral H211  C21  C22  C23 ! flat ? (180 degrees = trans)   177.47
! DIHEdral H212  C21  C22 H221 ! flat ? (180 degrees = trans)   172.56
! DIHEdral H212  C21  C22 H222 ! flexible dihedral ???    52.54
! DIHEdral H212  C21  C22  C23 ! flexible dihedral ???   -67.46
! DIHEdral  C21  C22  C23 H232 ! flexible dihedral ???   -80.13
! DIHEdral H222  C22  C23 H231 ! flexible dihedral ???   -84.41
! DIHEdral  C23  C24  C25 H252 ! flexible dihedral ???   -83.13
! DIHEdral H241  C24  C25  C26 ! flexible dihedral ???   -83.36
! DIHEdral H242  C24  C25 H251 ! flexible dihedral ???   -82.83
! DIHEdral  C24  C25  C26  C27 ! flexible dihedral ???    99.02
! DIHEdral H251  C25  C26 H261 ! flexible dihedral ???    99.35
! DIHEdral H252  C25  C26 H262 ! flexible dihedral ???    98.71
! DIHEdral  C25  C26  C27 H272 ! flat ? (0 degrees = cis)     0.46
! DIHEdral H261  C26  C27  C28 ! flat ? (0 degrees = cis)     2.95
! DIHEdral H262  C26  C27 H271 ! flat ? (0 degrees = cis)    -1.98
! DIHEdral  C26  C27  C28 H281 ! flat ? (180 degrees = trans)   179.98
! DIHEdral  C26  C27  C28 H282 ! flexible dihedral ???   -60.00
! DIHEdral  C26  C27  C28 H283 ! flexible dihedral ???    60.01
! DIHEdral H271  C27  C28 H281 ! flexible dihedral ???   -58.11
! DIHEdral H271  C27  C28 H282 ! flexible dihedral ???    61.91
! DIHEdral H271  C27  C28 H283 ! flat ? (180 degrees = trans)   181.92
! DIHEdral H272  C27  C28 H281 ! flexible dihedral ???    58.08
! DIHEdral H272  C27  C28 H282 ! flat ? (180 degrees = trans)   178.11
! DIHEdral H272  C27  C28 H283 ! flexible dihedral ???   -61.89
! DIHEdral  O2   C31  C32 H321 ! flat ? (0 degrees = cis)     0.31
! DIHEdral  O31  C31  C32 H321 ! flat ? (180 degrees = trans)   179.77
! DIHEdral  O31  C31  C32 H322 ! flexible dihedral ???    59.80
! DIHEdral  O31  C31  C32  C33 ! flexible dihedral ???   -60.19
! DIHEdral  C32  C31  O2   C2  ! flat ? (180 degrees = trans)   186.67
! DIHEdral  O31  C31  O2   C2  ! flat ? (0 degrees = cis)     7.25
! DIHEdral H321  C32  C33 H332 ! flat ? (0 degrees = cis)    -8.27
! DIHEdral  C32  C33  C34 H341 ! flexible dihedral ???    92.89
! DIHEdral H331  C33  C34 H342 ! flexible dihedral ???    94.15
! DIHEdral H332  C33  C34  C35 ! flexible dihedral ???    91.64
! DIHEdral H342  C34  C35 H352 ! flexible dihedral ???    96.42
! DIHEdral  C34  C35  C36 H362 ! flexible dihedral ???   -86.89
! DIHEdral H351  C35  C36  C37 ! flexible dihedral ???   -87.88
! DIHEdral H352  C35  C36 H361 ! flexible dihedral ???   -85.89
! DIHEdral  C35  C36  C37  C38 ! flexible dihedral ???   -91.03
! DIHEdral H361  C36  C37 H371 ! flexible dihedral ???   -86.62
! DIHEdral H362  C36  C37 H372 ! flexible dihedral ???   -95.38
! DIHEdral  C36  C37  C38 H382 ! flexible dihedral ???   -89.75
! DIHEdral H371  C37  C38  C39 ! flexible dihedral ???   -89.05
! DIHEdral H372  C37  C38 H381 ! flexible dihedral ???   -90.49
! DIHEdral  C37  C38  C39 H391 ! flexible dihedral ???    69.44
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! DIHEdral  C37  C38  C39 H392 ! flexible dihedral ???   -50.55
! DIHEdral  C37  C38  C39  C40 ! flat ? (180 degrees = trans)   189.47
! DIHEdral H382  C38  C39 H391 ! flexible dihedral ???   -51.66
! DIHEdral H382  C38  C39 H392 ! flat ? (180 degrees = trans)   188.35
! DIHEdral H382  C38  C39  C40 ! flexible dihedral ???    68.37
! DIHEdral  C38  C39  C40  C41 ! flat ? (0 degrees = cis)     0.17
! DIHEdral H391  C39  C40 H401 ! flat ? (0 degrees = cis)     0.70
! DIHEdral H392  C39  C40 H402 ! flat ? (0 degrees = cis)    -0.37
! DIHEdral H402  C40  C41 H411 ! flexible dihedral ???   -51.12
! DIHEdral H402  C40  C41 H412 ! flat ? (180 degrees = trans)   188.83
! DIHEdral H402  C40  C41  C42 ! flexible dihedral ???    68.86
! DIHEdral  C40  C41  C42 H421 ! flexible dihedral ???    94.94
! DIHEdral H411  C41  C42 H422 ! flexible dihedral ???    95.24
! DIHEdral H412  C41  C42  C43 ! flexible dihedral ???    94.59
! DIHEdral  C42  C43  C44  C45 ! flexible dihedral ???    90.47
! DIHEdral H431  C43  C44 H441 ! flexible dihedral ???    88.16
! DIHEdral H432  C43  C44 H442 ! flexible dihedral ???    92.82
! DIHEdral  C43  C44  C45 H452 ! flexible dihedral ???   -85.05
! DIHEdral H441  C44  C45  C46 ! flexible dihedral ???   -82.98
! DIHEdral H442  C44  C45 H451 ! flexible dihedral ???   -87.12
! DIHEdral  C45  C46  C47 H471 ! flexible dihedral ???    51.72
! DIHEdral  C45  C46  C47 H472 ! flexible dihedral ???   -68.27
! DIHEdral  C45  C46  C47  C48 ! flat ? (180 degrees = trans)   171.73
! DIHEdral H461  C46  C47 H471 ! flat ? (180 degrees = trans)   175.54
! DIHEdral H461  C46  C47 H472 ! flexible dihedral ???    55.55
! DIHEdral H461  C46  C47  C48 ! flexible dihedral ???   -64.44
! DIHEdral  C46  C47  C48 H481 ! flat ? (180 degrees = trans)   180.01
! DIHEdral  C46  C47  C48 H482 ! flexible dihedral ???   -59.99
! DIHEdral  C46  C47  C48 H483 ! flexible dihedral ???    59.98
! DIHEdral H471  C47  C48 H481 ! flexible dihedral ???   -61.34
! DIHEdral H471  C47  C48 H482 ! flexible dihedral ???    58.66
! DIHEdral H471  C47  C48 H483 ! flat ? (180 degrees = trans)   178.63
! DIHEdral H472  C47  C48 H481 ! flexible dihedral ???    61.37
! DIHEdral H472  C47  C48 H482 ! flat ? (180 degrees = trans)   181.37
! DIHEdral H472  C47  C48 H483 ! flexible dihedral ???   -58.66
! DIHEdral  C1   O3P  P    O2P ! flexible dihedral ???    83.90
! DIHEdral  C4   O4P  P    O1P ! flat ? (0 degrees = cis)    -6.97

 { edit these IMPRopers if necessary }
 IMPRoper  C1   H11  H12  C2  ! chirality or flatness improper    43.99
 IMPRoper  C2   C1   H2   C3  ! chirality or flatness improper    38.55
 IMPRoper  C3   C2   H31  H32 ! chirality or flatness improper    33.15
 IMPRoper  C4   H41  H42  C5  ! chirality or flatness improper    46.75
 IMPRoper  C5   C4   H51  H52 ! chirality or flatness improper    33.20
 IMPRoper  C6   H61  H62  H63 ! chirality or flatness improper    35.32
 IMPRoper  C7   H71  H72  H73 ! chirality or flatness improper    35.31
 IMPRoper  C8   H81  H82  H83 ! chirality or flatness improper    35.33
 IMPRoper  C11  C12  O3   O11 ! chirality or flatness improper     0.88
 IMPRoper  C12  C11 H121 H122 ! chirality or flatness improper    32.97
 IMPRoper  C13  C12 H131 H132 ! chirality or flatness improper    32.92
 IMPRoper  C14  C13 H141 H142 ! chirality or flatness improper    33.22
 IMPRoper  C15  C14 H151 H152 ! chirality or flatness improper    32.93
 IMPRoper  C16  C15 H161 H162 ! chirality or flatness improper    33.44
 IMPRoper  C17  C16 H171 H172 ! chirality or flatness improper    33.41
 IMPRoper  C18  C17 H181 H182 ! chirality or flatness improper    33.31
 IMPRoper  C19  C18 H191 H192 ! chirality or flatness improper    33.45
 IMPRoper  C20  C19 H201 H202 ! chirality or flatness improper    33.43
 IMPRoper  C21  C20 H211 H212 ! chirality or flatness improper    33.03
 IMPRoper  C22  C21 H221 H222 ! chirality or flatness improper    32.90
 IMPRoper  C23  C22 H231 H232 ! chirality or flatness improper    32.95
 IMPRoper  C24  C23 H241 H242 ! chirality or flatness improper    33.33
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 IMPRoper  C25  C24 H251 H252 ! chirality or flatness improper    33.40
 IMPRoper  C26  C25 H261 H262 ! chirality or flatness improper    33.09
 IMPRoper  C27  C26 H271 H272 ! chirality or flatness improper    33.07
 IMPRoper  C28  C27 H281 H282 ! chirality or flatness improper   -33.28
 IMPRoper  C31  C32  O2   O31 ! chirality or flatness improper    -0.27
 IMPRoper  C32  C31 H321 H322 ! chirality or flatness improper    33.08
 IMPRoper  C33  C32 H331 H332 ! chirality or flatness improper    33.25
 IMPRoper  C34  C33 H341 H342 ! chirality or flatness improper    33.06
 IMPRoper  C35  C34 H351 H352 ! chirality or flatness improper    33.38
 IMPRoper  C36  C35 H361 H362 ! chirality or flatness improper    32.97
 IMPRoper  C37  C36 H371 H372 ! chirality or flatness improper    33.33
 IMPRoper  C38  C37 H381 H382 ! chirality or flatness improper    33.23
 IMPRoper  C39  C38 H391 H392 ! chirality or flatness improper    33.49
 IMPRoper  C40  C39 H401 H402 ! chirality or flatness improper    33.10
 IMPRoper  C41  C40 H411 H412 ! chirality or flatness improper    33.36
 IMPRoper  C42  C41 H421 H422 ! chirality or flatness improper    32.98
 IMPRoper  C43  C42 H431 H432 ! chirality or flatness improper    33.57
 IMPRoper  C44  C43 H441 H442 ! chirality or flatness improper    33.22
 IMPRoper  C45  C44 H451 H452 ! chirality or flatness improper    33.29
 IMPRoper  C46  C45 H461 H462 ! chirality or flatness improper    33.04
 IMPRoper  C47  C46 H471 H472 ! chirality or flatness improper    33.44
 IMPRoper  C48  C47 H481 H482 ! chirality or flatness improper   -33.33
 IMPRoper  N    C5   C6   C7  ! chirality or flatness improper   -33.14
 IMPRoper  P    O1P  O2P  O3P ! chirality or flatness improper    34.95

 { edit any DONOrs and ACCEptors if necessary }
 ACCEptor  O2   C2
 ACCEptor  O3   C3
 ACCEptor  O11  C11
 ACCEptor  O31  C31
 ACCEptor  O1P  P
 ACCEptor  O2P  P
 ACCEptor  O3P  C1
 ACCEptor  O4P  C4

END { RESIdue PC2 }



PC2_par.txt
Remarks ../../tmp/hicup_btcpxq_9457/PC2_par.txt
Remarks Created by XPLO2D V. 001221/2.8.9 at Mon Apr 23 13:31:21 2001 for
A. Nonymous
Remarks Auto-generated by XPLO2D from file ../../tmp/hicup_btcpxq_
9457/user.pdb
Remarks Parameters for residue type PC2

 set echo=false end

 { edit if necessary }
 BOND CX1  HX2    1000.0  1.090 ! Nobs =    1
 BOND CX1  HX3    1000.0  1.090 ! Nobs =    1
 BOND CX1  CX4    1000.0  1.518 ! Nobs =    1
 BOND CX1  OX14   1000.0  1.449 ! Nobs =    1
 BOND CX4  HX5    1000.0  1.090 ! Nobs =    1
 BOND CX4  CX6    1000.0  1.548 ! Nobs =    1
 BOND CX4  OX13   1000.0  1.414 ! Nobs =    1
 BOND CX6  HX7    1000.0  1.090 ! Nobs =    1
 BOND CX6  HX8    1000.0  1.090 ! Nobs =    1
 BOND CX6  OX1A   1000.0  1.442 ! Nobs =    1
 BOND CX9  HX10   1000.0  1.090 ! Nobs =    1
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BOND CX9  HX11   1000.0  1.090 ! Nobs =    1
BOND CX9  CX12   1000.0  1.559 ! Nobs =    1
BOND CX9  OX1F   1000.0  1.426 ! Nobs =    1
BOND CX12 HX13   1000.0  1.090 ! Nobs =    1
BOND CX12 HX14   1000.0  1.090 ! Nobs =    1
BOND CX12 NX13   1000.0  1.518 ! Nobs =    1
BOND CX15 HX16   1000.0  1.090 ! Nobs =    1
BOND CX15 HX17   1000.0  1.090 ! Nobs =    1
BOND CX15 HX18   1000.0  1.090 ! Nobs =    1
BOND CX15 NX13   1000.0  1.494 ! Nobs =    1
BOND CX19 HX20   1000.0  1.090 ! Nobs =    1
BOND CX19 HX21   1000.0  1.090 ! Nobs =    1
BOND CX19 HX22   1000.0  1.091 ! Nobs =    1
BOND CX19 NX13   1000.0  1.507 ! Nobs =    1
BOND CX23 HX24   1000.0  1.090 ! Nobs =    1
BOND CX23 HX25   1000.0  1.090 ! Nobs =    1
BOND CX23 HX26   1000.0  1.090 ! Nobs =    1
BOND CX23 NX13   1000.0  1.483 ! Nobs =    1
BOND CX27 CX28   1000.0  1.526 ! Nobs =    1
BOND CX27 OX1A   1000.0  1.518 ! Nobs =    1
BOND CX27 OX1B   1000.0  1.242 ! Nobs =    1
BOND CX28 HX29   1000.0  1.090 ! Nobs =    1
BOND CX28 HX30   1000.0  1.090 ! Nobs =    1
BOND CX28 CX31   1000.0  1.534 ! Nobs =    1
BOND CX31 HX32   1000.0  1.090 ! Nobs =    1
BOND CX31 HX33   1000.0  1.090 ! Nobs =    1
BOND CX31 CX34   1000.0  1.534 ! Nobs =    1
BOND CX34 HX35   1000.0  1.090 ! Nobs =    1
BOND CX34 HX36   1000.0  1.090 ! Nobs =    1
BOND CX34 CX37   1000.0  1.524 ! Nobs =    1
BOND CX37 HX38   1000.0  1.090 ! Nobs =    1
BOND CX37 HX39   1000.0  1.090 ! Nobs =    1
BOND CX37 CX40   1000.0  1.520 ! Nobs =    1
BOND CX40 HX41   1000.0  1.090 ! Nobs =    1
BOND CX40 HX42   1000.0  1.090 ! Nobs =    1
BOND CX40 CX43   1000.0  1.532 ! Nobs =    1
BOND CX43 HX44   1000.0  1.090 ! Nobs =    1
BOND CX43 HX45   1000.0  1.090 ! Nobs =    1
BOND CX43 CX46   1000.0  1.528 ! Nobs =    1
BOND CX46 HX47   1000.0  1.090 ! Nobs =    1
BOND CX46 HX48   1000.0  1.091 ! Nobs =    1
BOND CX46 CX49   1000.0  1.533 ! Nobs =    1
BOND CX49 HX50   1000.0  1.090 ! Nobs =    1
BOND CX49 HX51   1000.0  1.090 ! Nobs =    1
BOND CX49 CX52   1000.0  1.547 ! Nobs =    1
BOND CX52 HX53   1000.0  1.090 ! Nobs =    1
BOND CX52 HX54   1000.0  1.090 ! Nobs =    1
BOND CX52 CX55   1000.0  1.554 ! Nobs =    1
BOND CX55 HX56   1000.0  1.090 ! Nobs =    1
BOND CX55 HX57   1000.0  1.090 ! Nobs =    1
BOND CX55 CX58   1000.0  1.549 ! Nobs =    1
BOND CX58 HX59   1000.0  1.090 ! Nobs =    1
BOND CX58 HX60   1000.0  1.090 ! Nobs =    1
BOND CX58 CX61   1000.0  1.536 ! Nobs =    1
BOND CX61 HX62   1000.0  1.091 ! Nobs =    1
BOND CX61 HX63   1000.0  1.090 ! Nobs =    1
BOND CX61 CX64   1000.0  1.530 ! Nobs =    1
BOND CX64 HX65   1000.0  1.090 ! Nobs =    1
BOND CX64 HX66   1000.0  1.090 ! Nobs =    1
BOND CX64 CX67   1000.0  1.529 ! Nobs =    1
BOND CX67 HX68   1000.0  1.089 ! Nobs =    1
```

```
BOND CX67 HX69   1000.0  1.090 ! Nobs =    1
BOND CX67 CX70   1000.0  1.539 ! Nobs =    1
BOND CX70 HX71   1000.0  1.090 ! Nobs =    1
BOND CX70 HX72   1000.0  1.090 ! Nobs =    1
BOND CX70 CX73   1000.0  1.552 ! Nobs =    1
BOND CX73 HX74   1000.0  1.090 ! Nobs =    1
BOND CX73 HX75   1000.0  1.090 ! Nobs =    1
BOND CX73 CX76   1000.0  1.532 ! Nobs =    1
BOND CX76 HX77   1000.0  1.090 ! Nobs =    1
BOND CX76 HX78   1000.0  1.090 ! Nobs =    1
BOND CX76 HX79   1000.0  1.090 ! Nobs =    1
BOND CX80 CX81   1000.0  1.512 ! Nobs =    1
BOND CX80 OX13   1000.0  1.525 ! Nobs =    1
BOND CX80 OX1C   1000.0  1.252 ! Nobs =    1
BOND CX81 HX82   1000.0  1.090 ! Nobs =    1
BOND CX81 HX83   1000.0  1.090 ! Nobs =    1
BOND CX81 CX84   1000.0  1.516 ! Nobs =    1
BOND CX84 HX85   1000.0  1.090 ! Nobs =    1
BOND CX84 HX86   1000.0  1.090 ! Nobs =    1
BOND CX84 CX87   1000.0  1.513 ! Nobs =    1
BOND CX87 HX88   1000.0  1.090 ! Nobs =    1
BOND CX87 HX89   1000.0  1.090 ! Nobs =    1
BOND CX87 CX90   1000.0  1.526 ! Nobs =    1
BOND CX90 HX91   1000.0  1.090 ! Nobs =    1
BOND CX90 HX92   1000.0  1.090 ! Nobs =    1
BOND CX90 CX93   1000.0  1.524 ! Nobs =    1
BOND CX93 HX94   1000.0  1.090 ! Nobs =    1
BOND CX93 HX95   1000.0  1.090 ! Nobs =    1
BOND CX93 CX96   1000.0  1.503 ! Nobs =    1
BOND CX96 HX97   1000.0  1.090 ! Nobs =    1
BOND CX96 HX98   1000.0  1.090 ! Nobs =    1
BOND CX96 CX99   1000.0  1.529 ! Nobs =    1
BOND CX99 HX1A   1000.0  1.090 ! Nobs =    1
BOND CX99 HX1B   1000.0  1.090 ! Nobs =    1
BOND CX99 CX10   1000.0  1.531 ! Nobs =    1
BOND CX10 HX1C   1000.0  1.090 ! Nobs =    1
BOND CX10 HX1D   1000.0  1.089 ! Nobs =    1
BOND CX10 CX1A   1000.0  1.556 ! Nobs =    1
BOND CX1A HX1E   1000.0  1.090 ! Nobs =    1
BOND CX1A HX1F   1000.0  1.090 ! Nobs =    1
BOND CX1A CX1B   1000.0  1.535 ! Nobs =    1
BOND CX1B HX1G   1000.0  1.090 ! Nobs =    1
BOND CX1B HX1H   1000.0  1.090 ! Nobs =    1
BOND CX1B CX11   1000.0  1.531 ! Nobs =    1
BOND CX11 HX1I   1000.0  1.090 ! Nobs =    1
BOND CX11 HX1J   1000.0  1.090 ! Nobs =    1
BOND CX11 CX1C   1000.0  1.508 ! Nobs =    1
BOND CX1C HX1K   1000.0  1.090 ! Nobs =    1
BOND CX1C HX1L   1000.0  1.090 ! Nobs =    1
BOND CX1C CX1D   1000.0  1.511 ! Nobs =    1
BOND CX1D HX1M   1000.0  1.090 ! Nobs =    1
BOND CX1D HX1N   1000.0  1.090 ! Nobs =    1
BOND CX1D CX1E   1000.0  1.518 ! Nobs =    1
BOND CX1E HX12   1000.0  1.090 ! Nobs =    1
BOND CX1E HX1O   1000.0  1.090 ! Nobs =    1
BOND CX1E CX1F   1000.0  1.519 ! Nobs =    1
BOND CX1F HX1P   1000.0  1.090 ! Nobs =    1
BOND CX1F HX1Q   1000.0  1.090 ! Nobs =    1
BOND CX1F CX1G   1000.0  1.521 ! Nobs =    1
BOND CX1G HX1R   1000.0  1.090 ! Nobs =    1
BOND CX1G HX1S   1000.0  1.090 ! Nobs =    1
```

```
BOND CX1G CX1H   1000.0  1.522 ! Nobs =    1
BOND CX1H HX1T   1000.0  1.090 ! Nobs =    1
BOND CX1H HX1U   1000.0  1.090 ! Nobs =    1
BOND CX1H HX1V   1000.0  1.090 ! Nobs =    1
BOND OX1D PX14   1000.0  1.456 ! Nobs =    1
BOND OX1E PX14   1000.0  1.481 ! Nobs =    1
BOND OX14 PX14   1000.0  1.620 ! Nobs =    1
BOND OX1F PX14   1000.0  1.612 ! Nobs =    1

{ edit if necessary }
ANGLe HX2  CX1  HX3     500.0   112.63 ! Nobs =    1
ANGLe HX2  CX1  CX4     500.0   106.07 ! Nobs =    1
ANGLe HX2  CX1  OX14    500.0   112.64 ! Nobs =    1
ANGLe HX3  CX1  CX4     500.0   106.08 ! Nobs =    1
ANGLe HX3  CX1  OX14    500.0   112.66 ! Nobs =    1
ANGLe CX4  CX1  OX14    500.0   106.07 ! Nobs =    1
ANGLe CX1  CX4  HX5     500.0   106.21 ! Nobs =    1
ANGLe CX1  CX4  CX6     500.0   106.22 ! Nobs =    1
ANGLe CX1  CX4  OX13    500.0   107.02 ! Nobs =    1
ANGLe HX5  CX4  CX6     500.0   112.51 ! Nobs =    1
ANGLe HX5  CX4  OX13    500.0   121.81 ! Nobs =    1
ANGLe CX6  CX4  OX13    500.0   102.08 ! Nobs =    1
ANGLe CX4  CX6  HX7     500.0   110.51 ! Nobs =    1
ANGLe CX4  CX6  HX8     500.0   110.51 ! Nobs =    1
ANGLe CX4  CX6  OX1A    500.0   110.51 ! Nobs =    1
ANGLe HX7  CX6  HX8     500.0   108.41 ! Nobs =    1
ANGLe HX7  CX6  OX1A    500.0   108.41 ! Nobs =    1
ANGLe HX8  CX6  OX1A    500.0   108.42 ! Nobs =    1
ANGLe HX10 CX9  HX11    500.0   114.03 ! Nobs =    1
ANGLe HX10 CX9  CX12    500.0   104.38 ! Nobs =    1
ANGLe HX10 CX9  OX1F    500.0   114.06 ! Nobs =    1
ANGLe HX11 CX9  CX12    500.0   104.39 ! Nobs =    1
ANGLe HX11 CX9  OX1F    500.0   114.03 ! Nobs =    1
ANGLe CX12 CX9  OX1F    500.0   104.39 ! Nobs =    1
ANGLe CX9  CX12 HX13    500.0   109.72 ! Nobs =    1
ANGLe CX9  CX12 HX14    500.0   109.73 ! Nobs =    1
ANGLe CX9  CX12 NX13    500.0   109.75 ! Nobs =    1
ANGLe HX13 CX12 HX14    500.0   109.20 ! Nobs =    1
ANGLe HX13 CX12 NX13    500.0   109.21 ! Nobs =    1
ANGLe HX14 CX12 NX13    500.0   109.21 ! Nobs =    1
ANGLe HX16 CX15 HX17    500.0   109.47 ! Nobs =    1
ANGLe HX16 CX15 HX18    500.0   109.44 ! Nobs =    1
ANGLe HX16 CX15 NX13    500.0   109.49 ! Nobs =    1
ANGLe HX17 CX15 HX18    500.0   109.42 ! Nobs =    1
ANGLe HX17 CX15 NX13    500.0   109.48 ! Nobs =    1
ANGLe HX18 CX15 NX13    500.0   109.53 ! Nobs =    1
ANGLe HX20 CX19 HX21    500.0   109.45 ! Nobs =    1
ANGLe HX20 CX19 HX22    500.0   109.42 ! Nobs =    1
ANGLe HX20 CX19 NX13    500.0   109.52 ! Nobs =    1
ANGLe HX21 CX19 HX22    500.0   109.47 ! Nobs =    1
ANGLe HX21 CX19 NX13    500.0   109.47 ! Nobs =    1
ANGLe HX22 CX19 NX13    500.0   109.50 ! Nobs =    1
ANGLe HX24 CX23 HX25    500.0   109.47 ! Nobs =    1
ANGLe HX24 CX23 HX26    500.0   109.41 ! Nobs =    1
ANGLe HX24 CX23 NX13    500.0   109.49 ! Nobs =    1
ANGLe HX25 CX23 HX26    500.0   109.44 ! Nobs =    1
ANGLe HX25 CX23 NX13    500.0   109.52 ! Nobs =    1
ANGLe HX26 CX23 NX13    500.0   109.50 ! Nobs =    1
ANGLe CX28 CX27 OX1A    500.0   114.28 ! Nobs =    1
ANGLe CX28 CX27 OX1B    500.0   120.60 ! Nobs =    1
ANGLe OX1A CX27 OX1B    500.0   125.10 ! Nobs =    1
```

```
ANGLe CX27 CX28 HX29    500.0   112.92 ! Nobs =    1
ANGLe CX27 CX28 HX30    500.0   112.96 ! Nobs =    1
ANGLe CX27 CX28 CX31    500.0   112.95 ! Nobs =    1
ANGLe HX29 CX28 HX30    500.0   105.81 ! Nobs =    1
ANGLe HX29 CX28 CX31    500.0   105.79 ! Nobs =    1
ANGLe HX30 CX28 CX31    500.0   105.76 ! Nobs =    1
ANGLe CX28 CX31 HX32    500.0   113.55 ! Nobs =    1
ANGLe CX28 CX31 HX33    500.0   113.52 ! Nobs =    1
ANGLe CX28 CX31 CX34    500.0   113.52 ! Nobs =    1
ANGLe HX32 CX31 HX33    500.0   105.13 ! Nobs =    1
ANGLe HX32 CX31 CX34    500.0   105.11 ! Nobs =    1
ANGLe HX33 CX31 CX34    500.0   105.12 ! Nobs =    1
ANGLe CX31 CX34 HX35    500.0   110.02 ! Nobs =    1
ANGLe CX31 CX34 HX36    500.0   110.04 ! Nobs =    1
ANGLe CX31 CX34 CX37    500.0   110.01 ! Nobs =    1
ANGLe HX35 CX34 HX36    500.0   108.93 ! Nobs =    1
ANGLe HX35 CX34 CX37    500.0   108.91 ! Nobs =    1
ANGLe HX36 CX34 CX37    500.0   108.91 ! Nobs =    1
ANGLe CX34 CX37 HX38    500.0   113.79 ! Nobs =    1
ANGLe CX34 CX37 HX39    500.0   113.79 ! Nobs =    1
ANGLe CX34 CX37 CX40    500.0   113.79 ! Nobs =    1
ANGLe HX38 CX37 HX39    500.0   104.82 ! Nobs =    1
ANGLe HX38 CX37 CX40    500.0   104.84 ! Nobs =    1
ANGLe HX39 CX37 CX40    500.0   104.82 ! Nobs =    1
ANGLe CX37 CX40 HX41    500.0   108.30 ! Nobs =    1
ANGLe CX37 CX40 HX42    500.0   108.29 ! Nobs =    1
ANGLe CX37 CX40 CX43    500.0   108.27 ! Nobs =    1
ANGLe HX41 CX40 HX42    500.0   110.64 ! Nobs =    1
ANGLe HX41 CX40 CX43    500.0   110.62 ! Nobs =    1
ANGLe HX42 CX40 CX43    500.0   110.63 ! Nobs =    1
ANGLe CX40 CX43 HX44    500.0   108.31 ! Nobs =    1
ANGLe CX40 CX43 HX45    500.0   108.34 ! Nobs =    1
ANGLe CX40 CX43 CX46    500.0   114.16 ! Nobs =    1
ANGLe HX44 CX43 HX45    500.0   110.56 ! Nobs =    1
ANGLe HX44 CX43 CX46    500.0   107.74 ! Nobs =    1
ANGLe HX45 CX43 CX46    500.0   107.72 ! Nobs =    1
ANGLe CX43 CX46 HX47    500.0   109.50 ! Nobs =    1
ANGLe CX43 CX46 HX48    500.0   109.52 ! Nobs =    1
ANGLe CX43 CX46 CX49    500.0   109.50 ! Nobs =    1
ANGLe HX47 CX46 HX48    500.0   109.43 ! Nobs =    1
ANGLe HX47 CX46 CX49    500.0   109.44 ! Nobs =    1
ANGLe HX48 CX46 CX49    500.0   109.44 ! Nobs =    1
ANGLe CX46 CX49 HX50    500.0   107.75 ! Nobs =    1
ANGLe CX46 CX49 HX51    500.0   107.76 ! Nobs =    1
ANGLe CX46 CX49 CX52    500.0   116.47 ! Nobs =    1
ANGLe HX50 CX49 HX51    500.0   111.12 ! Nobs =    1
ANGLe HX50 CX49 CX52    500.0   106.87 ! Nobs =    1
ANGLe HX51 CX49 CX52    500.0   106.90 ! Nobs =    1
ANGLe CX49 CX52 HX53    500.0   107.62 ! Nobs =    1
ANGLe CX49 CX52 HX54    500.0   107.62 ! Nobs =    1
ANGLe CX49 CX52 CX55    500.0   117.02 ! Nobs =    1
ANGLe HX53 CX52 HX54    500.0   111.25 ! Nobs =    1
ANGLe HX53 CX52 CX55    500.0   106.67 ! Nobs =    1
ANGLe HX54 CX52 CX55    500.0   106.69 ! Nobs =    1
ANGLe CX52 CX55 HX56    500.0   111.54 ! Nobs =    1
ANGLe CX52 CX55 HX57    500.0   111.57 ! Nobs =    1
ANGLe CX52 CX55 CX58    500.0   111.54 ! Nobs =    1
ANGLe HX56 CX55 HX57    500.0   107.32 ! Nobs =    1
ANGLe HX56 CX55 CX58    500.0   107.32 ! Nobs =    1
ANGLe HX57 CX55 CX58    500.0   107.30 ! Nobs =    1
ANGLe CX55 CX58 HX59    500.0   113.17 ! Nobs =    1
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```
ANGLe CX55 CX58 HX60    500.0   113.17 ! Nobs =    1
ANGLe CX55 CX58 CX61    500.0   113.15 ! Nobs =    1
ANGLe HX59 CX58 HX60    500.0   105.54 ! Nobs =    1
ANGLe HX59 CX58 CX61    500.0   105.53 ! Nobs =    1
ANGLe HX60 CX58 CX61    500.0   105.54 ! Nobs =    1
ANGLe CX58 CX61 HX62    500.0   113.09 ! Nobs =    1
ANGLe CX58 CX61 HX63    500.0   113.09 ! Nobs =    1
ANGLe CX58 CX61 CX64    500.0   113.09 ! Nobs =    1
ANGLe HX62 CX61 HX63    500.0   105.62 ! Nobs =    1
ANGLe HX62 CX61 CX64    500.0   105.63 ! Nobs =    1
ANGLe HX63 CX61 CX64    500.0   105.62 ! Nobs =    1
ANGLe CX61 CX64 HX65    500.0   109.26 ! Nobs =    1
ANGLe CX61 CX64 HX66    500.0   109.25 ! Nobs =    1
ANGLe CX61 CX64 CX67    500.0   109.25 ! Nobs =    1
ANGLe HX65 CX64 HX66    500.0   109.66 ! Nobs =    1
ANGLe HX65 CX64 CX67    500.0   109.70 ! Nobs =    1
ANGLe HX66 CX64 CX67    500.0   109.70 ! Nobs =    1
ANGLe CX64 CX67 HX68    500.0   108.42 ! Nobs =    1
ANGLe CX64 CX67 HX69    500.0   108.41 ! Nobs =    1
ANGLe CX64 CX67 CX70    500.0   113.86 ! Nobs =    1
ANGLe HX68 CX67 HX69    500.0   110.54 ! Nobs =    1
ANGLe HX68 CX67 CX70    500.0   107.81 ! Nobs =    1
ANGLe HX69 CX67 CX70    500.0   107.81 ! Nobs =    1
ANGLe CX67 CX70 HX71    500.0   111.55 ! Nobs =    1
ANGLe CX67 CX70 HX72    500.0   111.57 ! Nobs =    1
ANGLe CX67 CX70 CX73    500.0   111.57 ! Nobs =    1
ANGLe HX71 CX70 HX72    500.0   107.30 ! Nobs =    1
ANGLe HX71 CX70 CX73    500.0   107.30 ! Nobs =    1
ANGLe HX72 CX70 CX73    500.0   107.30 ! Nobs =    1
ANGLe CX70 CX73 HX74    500.0   111.08 ! Nobs =    1
ANGLe CX70 CX73 HX75    500.0   111.06 ! Nobs =    1
ANGLe CX70 CX73 CX76    500.0   111.09 ! Nobs =    1
ANGLe HX74 CX73 HX75    500.0   107.86 ! Nobs =    1
ANGLe HX74 CX73 CX76    500.0   107.80 ! Nobs =    1
ANGLe HX75 CX73 CX76    500.0   107.80 ! Nobs =    1
ANGLe CX73 CX76 HX77    500.0   109.51 ! Nobs =    1
ANGLe CX73 CX76 HX78    500.0   109.51 ! Nobs =    1
ANGLe CX73 CX76 HX79    500.0   109.50 ! Nobs =    1
ANGLe HX77 CX76 HX78    500.0   109.45 ! Nobs =    1
ANGLe HX77 CX76 HX79    500.0   109.42 ! Nobs =    1
ANGLe HX78 CX76 HX79    500.0   109.44 ! Nobs =    1
ANGLe CX81 CX80 OX13    500.0   111.05 ! Nobs =    1
ANGLe CX81 CX80 OX1C    500.0   121.61 ! Nobs =    1
ANGLe OX13 CX80 OX1C    500.0   127.35 ! Nobs =    1
ANGLe CX80 CX81 HX82    500.0   112.74 ! Nobs =    1
ANGLe CX80 CX81 HX83    500.0   112.72 ! Nobs =    1
ANGLe CX80 CX81 CX84    500.0   112.73 ! Nobs =    1
ANGLe HX82 CX81 HX83    500.0   106.01 ! Nobs =    1
ANGLe HX82 CX81 CX84    500.0   106.05 ! Nobs =    1
ANGLe HX83 CX81 CX84    500.0   106.02 ! Nobs =    1
ANGLe CX81 CX84 HX85    500.0   110.51 ! Nobs =    1
ANGLe CX81 CX84 HX86    500.0   110.51 ! Nobs =    1
ANGLe CX81 CX84 CX87    500.0   110.52 ! Nobs =    1
ANGLe HX85 CX84 HX86    500.0   108.41 ! Nobs =    1
ANGLe HX85 CX84 CX87    500.0   108.39 ! Nobs =    1
ANGLe HX86 CX84 CX87    500.0   108.43 ! Nobs =    1
ANGLe CX84 CX87 HX88    500.0   112.60 ! Nobs =    1
ANGLe CX84 CX87 HX89    500.0   112.63 ! Nobs =    1
ANGLe CX84 CX87 CX90    500.0   112.61 ! Nobs =    1
ANGLe HX88 CX87 HX89    500.0   106.14 ! Nobs =    1
ANGLe HX88 CX87 CX90    500.0   106.18 ! Nobs =    1
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```
ANGLe HX89 CX87 CX90    500.0   106.14 ! Nobs =    1
ANGLe CX87 CX90 HX91    500.0   108.69 ! Nobs =    1
ANGLe CX87 CX90 HX92    500.0   108.66 ! Nobs =    1
ANGLe CX87 CX90 CX93    500.0   108.67 ! Nobs =    1
ANGLe HX91 CX90 HX92    500.0   110.27 ! Nobs =    1
ANGLe HX91 CX90 CX93    500.0   110.25 ! Nobs =    1
ANGLe HX92 CX90 CX93    500.0   110.25 ! Nobs =    1
ANGLe CX90 CX93 HX94    500.0   113.27 ! Nobs =    1
ANGLe CX90 CX93 HX95    500.0   113.26 ! Nobs =    1
ANGLe CX90 CX93 CX96    500.0   113.25 ! Nobs =    1
ANGLe HX94 CX93 HX95    500.0   105.42 ! Nobs =    1
ANGLe HX94 CX93 CX96    500.0   105.42 ! Nobs =    1
ANGLe HX95 CX93 CX96    500.0   105.44 ! Nobs =    1
ANGLe CX93 CX96 HX97    500.0   110.07 ! Nobs =    1
ANGLe CX93 CX96 HX98    500.0   110.06 ! Nobs =    1
ANGLe CX93 CX96 CX99    500.0   110.06 ! Nobs =    1
ANGLe HX97 CX96 HX98    500.0   108.87 ! Nobs =    1
ANGLe HX97 CX96 CX99    500.0   108.85 ! Nobs =    1
ANGLe HX98 CX96 CX99    500.0   108.90 ! Nobs =    1
ANGLe CX96 CX99 HX1A    500.0   110.39 ! Nobs =    1
ANGLe CX96 CX99 HX1B    500.0   110.37 ! Nobs =    1
ANGLe CX96 CX99 CX10    500.0   110.39 ! Nobs =    1
ANGLe HX1A CX99 HX1B    500.0   108.54 ! Nobs =    1
ANGLe HX1A CX99 CX10    500.0   108.54 ! Nobs =    1
ANGLe HX1B CX99 CX10    500.0   108.55 ! Nobs =    1
ANGLe CX99 CX10 HX1C    500.0   107.39 ! Nobs =    1
ANGLe CX99 CX10 HX1D    500.0   107.42 ! Nobs =    1
ANGLe CX99 CX10 CX1A    500.0   117.89 ! Nobs =    1
ANGLe HX1C CX10 HX1D    500.0   111.45 ! Nobs =    1
ANGLe HX1C CX10 CX1A    500.0   106.40 ! Nobs =    1
ANGLe HX1D CX10 CX1A    500.0   106.35 ! Nobs =    1
ANGLe CX10 CX1A HX1E    500.0   110.95 ! Nobs =    1
ANGLe CX10 CX1A HX1F    500.0   110.93 ! Nobs =    1
ANGLe CX10 CX1A CX1B    500.0   110.94 ! Nobs =    1
ANGLe HX1E CX1A HX1F    500.0   107.95 ! Nobs =    1
ANGLe HX1E CX1A CX1B    500.0   107.98 ! Nobs =    1
ANGLe HX1F CX1A CX1B    500.0   107.96 ! Nobs =    1
ANGLe CX1A CX1B HX1G    500.0   108.29 ! Nobs =    1
ANGLe CX1A CX1B HX1H    500.0   108.32 ! Nobs =    1
ANGLe CX1A CX1B CX11    500.0   114.27 ! Nobs =    1
ANGLe HX1G CX1B HX1H    500.0   110.65 ! Nobs =    1
ANGLe HX1G CX1B CX11    500.0   107.67 ! Nobs =    1
ANGLe HX1H CX1B CX11    500.0   107.64 ! Nobs =    1
ANGLe CX1B CX11 HX1I    500.0   112.96 ! Nobs =    1
ANGLe CX1B CX11 HX1J    500.0   112.93 ! Nobs =    1
ANGLe CX1B CX11 CX1C    500.0   112.95 ! Nobs =    1
ANGLe HX1I CX11 HX1J    500.0   105.81 ! Nobs =    1
ANGLe HX1I CX11 CX1C    500.0   105.77 ! Nobs =    1
ANGLe HX1J CX11 CX1C    500.0   105.78 ! Nobs =    1
ANGLe CX11 CX1C HX1K    500.0   107.65 ! Nobs =    1
ANGLe CX11 CX1C HX1L    500.0   107.62 ! Nobs =    1
ANGLe CX11 CX1C CX1D    500.0   107.64 ! Nobs =    1
ANGLe HX1K CX1C HX1L    500.0   111.23 ! Nobs =    1
ANGLe HX1K CX1C CX1D    500.0   111.25 ! Nobs =    1
ANGLe HX1L CX1C CX1D    500.0   111.24 ! Nobs =    1
ANGLe CX1C CX1D HX1M    500.0   111.20 ! Nobs =    1
ANGLe CX1C CX1D HX1N    500.0   111.20 ! Nobs =    1
ANGLe CX1C CX1D CX1E    500.0   111.18 ! Nobs =    1
ANGLe HX1M CX1D HX1N    500.0   107.65 ! Nobs =    1
ANGLe HX1M CX1D CX1E    500.0   107.72 ! Nobs =    1
ANGLe HX1N CX1D CX1E    500.0   107.71 ! Nobs =    1
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 ANGLe CX1D CX1E HX12    500.0   110.05 ! Nobs =    1
 ANGLe CX1D CX1E HX1O    500.0   110.05 ! Nobs =    1
 ANGLe CX1D CX1E CX1F    500.0   110.05 ! Nobs =    1
 ANGLe HX12 CX1E HX1O    500.0   108.89 ! Nobs =    1
 ANGLe HX12 CX1E CX1F    500.0   108.89 ! Nobs =    1
 ANGLe HX1O CX1E CX1F    500.0   108.88 ! Nobs =    1
 ANGLe CX1E CX1F HX1P    500.0   112.76 ! Nobs =    1
 ANGLe CX1E CX1F HX1Q    500.0   112.75 ! Nobs =    1
 ANGLe CX1E CX1F CX1G    500.0   112.76 ! Nobs =    1
 ANGLe HX1P CX1F HX1Q    500.0   105.99 ! Nobs =    1
 ANGLe HX1P CX1F CX1G    500.0   106.00 ! Nobs =    1
 ANGLe HX1Q CX1F CX1G    500.0   106.00 ! Nobs =    1
 ANGLe CX1F CX1G HX1R    500.0   108.38 ! Nobs =    1
 ANGLe CX1F CX1G HX1S    500.0   108.38 ! Nobs =    1
 ANGLe CX1F CX1G CX1H    500.0   108.38 ! Nobs =    1
 ANGLe HX1R CX1G HX1S    500.0   110.53 ! Nobs =    1
 ANGLe HX1R CX1G CX1H    500.0   110.55 ! Nobs =    1
 ANGLe HX1S CX1G CX1H    500.0   110.54 ! Nobs =    1
 ANGLe CX1G CX1H HX1T    500.0   109.54 ! Nobs =    1
 ANGLe CX1G CX1H HX1U    500.0   109.52 ! Nobs =    1
 ANGLe CX1G CX1H HX1V    500.0   109.47 ! Nobs =    1
 ANGLe HX1T CX1H HX1U    500.0   109.42 ! Nobs =    1
 ANGLe HX1T CX1H HX1V    500.0   109.46 ! Nobs =    1
 ANGLe HX1U CX1H HX1V    500.0   109.43 ! Nobs =    1
 ANGLe CX12 NX13 CX15    500.0   110.35 ! Nobs =    1
 ANGLe CX12 NX13 CX19    500.0   112.26 ! Nobs =    1
 ANGLe CX12 NX13 CX23    500.0   108.49 ! Nobs =    1
 ANGLe CX15 NX13 CX19    500.0   109.56 ! Nobs =    1
 ANGLe CX15 NX13 CX23    500.0   108.04 ! Nobs =    1
 ANGLe CX19 NX13 CX23    500.0   108.03 ! Nobs =    1
 ANGLe CX4  OX13 CX80    500.0   112.57 ! Nobs =    1
 ANGLe CX6  OX1A CX27    500.0   110.76 ! Nobs =    1
 ANGLe CX1  OX14 PX14    500.0   117.77 ! Nobs =    1
 ANGLe CX9  OX1F PX14    500.0   119.27 ! Nobs =    1
 ANGLe OX1D PX14 OX1E    500.0   113.64 ! Nobs =    1
 ANGLe OX1D PX14 OX14    500.0   107.09 ! Nobs =    1
 ANGLe OX1D PX14 OX1F    500.0   110.38 ! Nobs =    1
 ANGLe OX1E PX14 OX14    500.0   112.76 ! Nobs =    1
 ANGLe OX1E PX14 OX1F    500.0   110.49 ! Nobs =    1
 ANGLe OX14 PX14 OX1F    500.0   101.81 ! Nobs =    1

 { edit if necessary }
 DIHEdral HX2  CX1  CX4  OX13    750.0 0    90.00 ! Nobs =    1 ... Value =
86.47
 DIHEdral HX2  CX1  OX14 PX14    750.0 0   -60.00 ! Nobs =    1 ... Value =
-69.40
 DIHEdral HX3  CX1  OX14 PX14    750.0 0    60.00 ! Nobs =    1 ... Value =
59.35
 DIHEdral CX4  CX1  OX14 PX14    750.0 0   180.00 ! Nobs =    1 ... Value =
174.98
 DIHEdral CX1  CX4  CX6  HX8     750.0 0    90.00 ! Nobs =    1 ... Value =
89.50
 DIHEdral HX5  CX4  CX6  HX7     750.0 0    90.00 ! Nobs =    1 ... Value =
93.69
 DIHEdral OX13 CX4  CX6  OX1A    750.0 0    90.00 ! Nobs =    1 ... Value =
81.45
 DIHEdral CX4  CX6  OX1A CX27    750.0 0   180.00 ! Nobs =    1 ... Value =
179.15
 DIHEdral HX7  CX6  OX1A CX27    750.0 0   -60.00 ! Nobs =    1 ... Value =
-59.60
 DIHEdral HX8  CX6  OX1A CX27    750.0 0    60.00 ! Nobs =    1 ... Value =
```

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57.89
 DIHEdral HX10 CX9  CX12 HX13    750.0 0   -90.00 ! Nobs =    1 ... Value =
-97.33
 DIHEdral HX11 CX9  CX12 NX13    750.0 0   -90.00 ! Nobs =    1 ... Value =
-97.31
 DIHEdral OX1F CX9  CX12 HX14    750.0 0   -90.00 ! Nobs =    1 ... Value =
-97.29
 DIHEdral HX10 CX9  OX1F PX14    750.0 0   -60.00 ! Nobs =    1 ... Value =
-53.67
 DIHEdral CX9  CX12 NX13 CX15    750.0 0   -60.00 ! Nobs =    1 ... Value =
-62.17
 DIHEdral CX9  CX12 NX13 CX19    750.0 0    60.00 ! Nobs =    1 ... Value =
60.35
 DIHEdral CX9  CX12 NX13 CX23    750.0 0   180.00 ! Nobs =    1 ... Value =
179.65
 DIHEdral HX13 CX12 NX13 CX15    750.0 0    60.00 ! Nobs =    1 ... Value =
58.15
 DIHEdral HX13 CX12 NX13 CX19    750.0 0   180.00 ! Nobs =    1 ... Value =
-179.33
 DIHEdral HX13 CX12 NX13 CX23    750.0 0   -60.00 ! Nobs =    1 ... Value =
-60.03
 DIHEdral HX14 CX12 NX13 CX15    750.0 0   180.00 ! Nobs =    1 ... Value =
177.50
 DIHEdral HX14 CX12 NX13 CX19    750.0 0   -60.00 ! Nobs =    1 ... Value =
-59.98
 DIHEdral HX14 CX12 NX13 CX23    750.0 0    60.00 ! Nobs =    1 ... Value =
59.32
 DIHEdral HX16 CX15 NX13 CX12    750.0 0   180.00 ! Nobs =    1 ... Value =
-180.00
 DIHEdral HX16 CX15 NX13 CX19    750.0 0    60.00 ! Nobs =    1 ... Value =
55.92
 DIHEdral HX16 CX15 NX13 CX23    750.0 0   -60.00 ! Nobs =    1 ... Value =
-61.55
 DIHEdral HX17 CX15 NX13 CX12    750.0 0   -60.00 ! Nobs =    1 ... Value =
-59.98
 DIHEdral HX17 CX15 NX13 CX19    750.0 0   180.00 ! Nobs =    1 ... Value =
175.94
 DIHEdral HX17 CX15 NX13 CX23    750.0 0    60.00 ! Nobs =    1 ... Value =
58.47
 DIHEdral HX18 CX15 NX13 CX12    750.0 0    60.00 ! Nobs =    1 ... Value =
60.00
 DIHEdral HX18 CX15 NX13 CX19    750.0 0   -60.00 ! Nobs =    1 ... Value =
-64.09
 DIHEdral HX18 CX15 NX13 CX23    750.0 0   180.00 ! Nobs =    1 ... Value =
178.45
 DIHEdral HX20 CX19 NX13 CX12    750.0 0   180.00 ! Nobs =    1 ... Value =
179.99
 DIHEdral HX20 CX19 NX13 CX15    750.0 0   -60.00 ! Nobs =    1 ... Value =
-57.04
 DIHEdral HX20 CX19 NX13 CX23    750.0 0    60.00 ! Nobs =    1 ... Value =
60.42
 DIHEdral HX21 CX19 NX13 CX12    750.0 0   -60.00 ! Nobs =    1 ... Value =
-60.00
 DIHEdral HX21 CX19 NX13 CX15    750.0 0    60.00 ! Nobs =    1 ... Value =
62.96
 DIHEdral HX21 CX19 NX13 CX23    750.0 0   180.00 ! Nobs =    1 ... Value =
-179.58
 DIHEdral HX22 CX19 NX13 CX12    750.0 0    60.00 ! Nobs =    1 ... Value =
60.02
 DIHEdral HX22 CX19 NX13 CX15    750.0 0   180.00 ! Nobs =    1 ... Value =
-177.02
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 DIHEdral HX22 CX19 NX13 CX23    750.0 0   -60.00 ! Nobs =    1 ... Value =
-59.56
 DIHEdral HX24 CX23 NX13 CX12    750.0 0   180.00 ! Nobs =    1 ... Value =
179.98
 DIHEdral HX24 CX23 NX13 CX15    750.0 0    60.00 ! Nobs =    1 ... Value =
60.34
 DIHEdral HX24 CX23 NX13 CX19    750.0 0   -60.00 ! Nobs =    1 ... Value =
-58.10
 DIHEdral HX25 CX23 NX13 CX12    750.0 0   -60.00 ! Nobs =    1 ... Value =
-59.99
 DIHEdral HX25 CX23 NX13 CX15    750.0 0   180.00 ! Nobs =    1 ... Value =
-179.62
 DIHEdral HX25 CX23 NX13 CX19    750.0 0    60.00 ! Nobs =    1 ... Value =
61.94
 DIHEdral HX26 CX23 NX13 CX12    750.0 0    60.00 ! Nobs =    1 ... Value =
60.02
 DIHEdral HX26 CX23 NX13 CX15    750.0 0   -60.00 ! Nobs =    1 ... Value =
-59.61
 DIHEdral HX26 CX23 NX13 CX19    750.0 0   180.00 ! Nobs =    1 ... Value =
-178.05
 DIHEdral OX1A CX27 CX28 HX30    750.0 0    90.00 ! Nobs =    1 ... Value =
89.54
 DIHEdral OX1B CX27 CX28 HX30    750.0 0   -90.00 ! Nobs =    1 ... Value =
-88.76
 DIHEdral CX27 CX28 CX31 CX34    750.0 0   -90.00 ! Nobs =    1 ... Value =
-87.15
 DIHEdral HX29 CX28 CX31 HX32    750.0 0   -90.00 ! Nobs =    1 ... Value =
-83.14
 DIHEdral HX30 CX28 CX31 HX33    750.0 0   -90.00 ! Nobs =    1 ... Value =
-91.20
 DIHEdral CX28 CX31 CX34 HX35    750.0 0    90.00 ! Nobs =    1 ... Value =
97.07
 DIHEdral HX33 CX31 CX34 CX37    750.0 0    90.00 ! Nobs =    1 ... Value =
92.41
 DIHEdral HX38 CX37 CX40 CX43    750.0 0   -90.00 ! Nobs =    1 ... Value =
-97.50
 DIHEdral CX40 CX43 CX46 CX49    750.0 0    90.00 ! Nobs =    1 ... Value =
83.54
 DIHEdral HX44 CX43 CX46 HX47    750.0 0    90.00 ! Nobs =    1 ... Value =
83.88
 DIHEdral HX45 CX43 CX46 HX48    750.0 0    90.00 ! Nobs =    1 ... Value =
83.18
 DIHEdral CX43 CX46 CX49 HX50    750.0 0    60.00 ! Nobs =    1 ... Value =
62.68
 DIHEdral CX43 CX46 CX49 HX51    750.0 0   -60.00 ! Nobs =    1 ... Value =
-57.30
 DIHEdral CX43 CX46 CX49 CX52    750.0 0   180.00 ! Nobs =    1 ... Value =
-177.34
 DIHEdral HX47 CX46 CX49 HX50    750.0 0   180.00 ! Nobs =    1 ... Value =
-177.28
 DIHEdral HX47 CX46 CX49 HX51    750.0 0    60.00 ! Nobs =    1 ... Value =
62.73
 DIHEdral HX47 CX46 CX49 CX52    750.0 0   -60.00 ! Nobs =    1 ... Value =
-57.30
 DIHEdral HX48 CX46 CX49 HX50    750.0 0   -60.00 ! Nobs =    1 ... Value =
-57.37
 DIHEdral HX48 CX46 CX49 HX51    750.0 0   180.00 ! Nobs =    1 ... Value =
-177.36
 DIHEdral HX48 CX46 CX49 CX52    750.0 0    60.00 ! Nobs =    1 ... Value =
62.61
 DIHEdral CX46 CX49 CX52 CX55    750.0 0     0.00 ! Nobs =    1 ... Value =
```

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-0.03
 DIHEdral HX50 CX49 CX52 HX53    750.0 0     0.00 ! Nobs =    1 ... Value =
0.43
 DIHEdral HX51 CX49 CX52 HX54    750.0 0     0.00 ! Nobs =    1 ... Value =
-0.51
 DIHEdral CX52 CX55 CX58 HX59    750.0 0   -60.00 ! Nobs =    1 ... Value =
-64.97
 DIHEdral CX52 CX55 CX58 HX60    750.0 0   180.00 ! Nobs =    1 ... Value =
175.02
 DIHEdral CX52 CX55 CX58 CX61    750.0 0    60.00 ! Nobs =    1 ... Value =
55.02
 DIHEdral HX56 CX55 CX58 HX59    750.0 0    60.00 ! Nobs =    1 ... Value =
57.48
 DIHEdral HX56 CX55 CX58 HX60    750.0 0   -60.00 ! Nobs =    1 ... Value =
-62.53
 DIHEdral HX56 CX55 CX58 CX61    750.0 0   180.00 ! Nobs =    1 ... Value =
177.47
 DIHEdral HX57 CX55 CX58 HX59    750.0 0   180.00 ! Nobs =    1 ... Value =
172.56
 DIHEdral HX57 CX55 CX58 HX60    750.0 0    60.00 ! Nobs =    1 ... Value =
52.54
 DIHEdral HX57 CX55 CX58 CX61    750.0 0   -60.00 ! Nobs =    1 ... Value =
-67.46
 DIHEdral CX55 CX58 CX61 HX63    750.0 0   -90.00 ! Nobs =    1 ... Value =
-80.13
 DIHEdral HX60 CX58 CX61 HX62    750.0 0   -90.00 ! Nobs =    1 ... Value =
-84.41
 DIHEdral CX61 CX64 CX67 HX69    750.0 0   -90.00 ! Nobs =    1 ... Value =
-83.13
 DIHEdral HX65 CX64 CX67 CX70    750.0 0   -90.00 ! Nobs =    1 ... Value =
-83.36
 DIHEdral HX66 CX64 CX67 HX68    750.0 0   -90.00 ! Nobs =    1 ... Value =
-82.83
 DIHEdral CX64 CX67 CX70 CX73    750.0 0    90.00 ! Nobs =    1 ... Value =
99.02
 DIHEdral HX68 CX67 CX70 HX71    750.0 0    90.00 ! Nobs =    1 ... Value =
99.35
 DIHEdral HX69 CX67 CX70 HX72    750.0 0    90.00 ! Nobs =    1 ... Value =
98.71
 DIHEdral CX67 CX70 CX73 HX75    750.0 0     0.00 ! Nobs =    1 ... Value =
0.46
 DIHEdral HX71 CX70 CX73 CX76    750.0 0     0.00 ! Nobs =    1 ... Value =
2.95
 DIHEdral HX72 CX70 CX73 HX74    750.0 0     0.00 ! Nobs =    1 ... Value =
-1.98
 DIHEdral CX70 CX73 CX76 HX77    750.0 0   180.00 ! Nobs =    1 ... Value =
179.98
 DIHEdral CX70 CX73 CX76 HX78    750.0 0   -60.00 ! Nobs =    1 ... Value =
-60.00
 DIHEdral CX70 CX73 CX76 HX79    750.0 0    60.00 ! Nobs =    1 ... Value =
60.01
 DIHEdral HX74 CX73 CX76 HX77    750.0 0   -60.00 ! Nobs =    1 ... Value =
-58.11
 DIHEdral HX74 CX73 CX76 HX78    750.0 0    60.00 ! Nobs =    1 ... Value =
61.91
 DIHEdral HX74 CX73 CX76 HX79    750.0 0   180.00 ! Nobs =    1 ... Value =
-178.08
 DIHEdral HX75 CX73 CX76 HX77    750.0 0    60.00 ! Nobs =    1 ... Value =
58.08
 DIHEdral HX75 CX73 CX76 HX78    750.0 0   180.00 ! Nobs =    1 ... Value =
178.11
```

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 DIHEdral HX75 CX73 CX76 HX79    750.0 0   -60.00 ! Nobs =    1 ... Value =
-61.89
 DIHEdral OX13 CX80 CX81 HX82    750.0 0     0.00 ! Nobs =    1 ... Value =
0.31
 DIHEdral OX1C CX80 CX81 HX82    750.0 0   180.00 ! Nobs =    1 ... Value =
179.77
 DIHEdral OX1C CX80 CX81 HX83    750.0 0    60.00 ! Nobs =    1 ... Value =
59.80
 DIHEdral OX1C CX80 CX81 CX84    750.0 0   -60.00 ! Nobs =    1 ... Value =
-60.19
 DIHEdral CX81 CX80 OX13 CX4     750.0 0   180.00 ! Nobs =    1 ... Value =
-173.33
 DIHEdral OX1C CX80 OX13 CX4     750.0 0     0.00 ! Nobs =    1 ... Value =
7.25
 DIHEdral HX82 CX81 CX84 HX86    750.0 0     0.00 ! Nobs =    1 ... Value =
-8.27
 DIHEdral CX81 CX84 CX87 HX88    750.0 0    90.00 ! Nobs =    1 ... Value =
92.89
 DIHEdral HX85 CX84 CX87 HX89    750.0 0    90.00 ! Nobs =    1 ... Value =
94.15
 DIHEdral HX86 CX84 CX87 CX90    750.0 0    90.00 ! Nobs =    1 ... Value =
91.64
 DIHEdral HX89 CX87 CX90 HX92    750.0 0    90.00 ! Nobs =    1 ... Value =
96.42
 DIHEdral CX87 CX90 CX93 HX95    750.0 0   -90.00 ! Nobs =    1 ... Value =
-86.89
 DIHEdral HX91 CX90 CX93 CX96    750.0 0   -90.00 ! Nobs =    1 ... Value =
-87.88
 DIHEdral HX92 CX90 CX93 HX94    750.0 0   -90.00 ! Nobs =    1 ... Value =
-85.89
 DIHEdral CX90 CX93 CX96 CX99    750.0 0   -90.00 ! Nobs =    1 ... Value =
-91.03
 DIHEdral HX94 CX93 CX96 HX97    750.0 0   -90.00 ! Nobs =    1 ... Value =
-86.62
 DIHEdral HX95 CX93 CX96 HX98    750.0 0   -90.00 ! Nobs =    1 ... Value =
-95.38
 DIHEdral CX93 CX96 CX99 HX1B    750.0 0   -90.00 ! Nobs =    1 ... Value =
-89.75
 DIHEdral HX97 CX96 CX99 CX10    750.0 0   -90.00 ! Nobs =    1 ... Value =
-89.05
 DIHEdral HX98 CX96 CX99 HX1A    750.0 0   -90.00 ! Nobs =    1 ... Value =
-90.49
 DIHEdral CX96 CX99 CX10 HX1C    750.0 0    60.00 ! Nobs =    1 ... Value =
69.44
 DIHEdral CX96 CX99 CX10 HX1D    750.0 0   -60.00 ! Nobs =    1 ... Value =
-50.55
 DIHEdral CX96 CX99 CX10 CX1A    750.0 0   180.00 ! Nobs =    1 ... Value =
-170.53
 DIHEdral HX1B CX99 CX10 HX1C    750.0 0   -60.00 ! Nobs =    1 ... Value =
-51.66
 DIHEdral HX1B CX99 CX10 HX1D    750.0 0   180.00 ! Nobs =    1 ... Value =
-171.65
 DIHEdral HX1B CX99 CX10 CX1A    750.0 0    60.00 ! Nobs =    1 ... Value =
68.37
 DIHEdral CX99 CX10 CX1A CX1B    750.0 0     0.00 ! Nobs =    1 ... Value =
0.17
 DIHEdral HX1C CX10 CX1A HX1E    750.0 0     0.00 ! Nobs =    1 ... Value =
0.70
 DIHEdral HX1D CX10 CX1A HX1F    750.0 0     0.00 ! Nobs =    1 ... Value =
-0.37
 DIHEdral HX1F CX1A CX1B HX1G    750.0 0   -60.00 ! Nobs =    1 ... Value =
```

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-51.12
 DIHEdral HX1F CX1A CX1B HX1H    750.0 0   180.00 ! Nobs =    1 ... Value =
-171.17
 DIHEdral HX1F CX1A CX1B CX11    750.0 0    60.00 ! Nobs =    1 ... Value =
68.86
 DIHEdral CX1A CX1B CX11 HX1I    750.0 0    90.00 ! Nobs =    1 ... Value =
94.94
 DIHEdral HX1G CX1B CX11 HX1J    750.0 0    90.00 ! Nobs =    1 ... Value =
95.24
 DIHEdral HX1H CX1B CX11 CX1C    750.0 0    90.00 ! Nobs =    1 ... Value =
94.59
 DIHEdral CX11 CX1C CX1D CX1E    750.0 0    90.00 ! Nobs =    1 ... Value =
90.47
 DIHEdral HX1K CX1C CX1D HX1M    750.0 0    90.00 ! Nobs =    1 ... Value =
88.16
 DIHEdral HX1L CX1C CX1D HX1N    750.0 0    90.00 ! Nobs =    1 ... Value =
92.82
 DIHEdral CX1C CX1D CX1E HX1O    750.0 0   -90.00 ! Nobs =    1 ... Value =
-85.05
 DIHEdral HX1M CX1D CX1E CX1F    750.0 0   -90.00 ! Nobs =    1 ... Value =
-82.98
 DIHEdral HX1N CX1D CX1E HX12    750.0 0   -90.00 ! Nobs =    1 ... Value =
-87.12
 DIHEdral CX1E CX1F CX1G HX1R    750.0 0    60.00 ! Nobs =    1 ... Value =
51.72
 DIHEdral CX1E CX1F CX1G HX1S    750.0 0   -60.00 ! Nobs =    1 ... Value =
-68.27
 DIHEdral CX1E CX1F CX1G CX1H    750.0 0   180.00 ! Nobs =    1 ... Value =
171.73
 DIHEdral HX1P CX1F CX1G HX1R    750.0 0   180.00 ! Nobs =    1 ... Value =
175.54
 DIHEdral HX1P CX1F CX1G HX1S    750.0 0    60.00 ! Nobs =    1 ... Value =
55.55
 DIHEdral HX1P CX1F CX1G CX1H    750.0 0   -60.00 ! Nobs =    1 ... Value =
-64.44
 DIHEdral CX1F CX1G CX1H HX1T    750.0 0   180.00 ! Nobs =    1 ... Value =
-179.99
 DIHEdral CX1F CX1G CX1H HX1U    750.0 0   -60.00 ! Nobs =    1 ... Value =
-59.99
 DIHEdral CX1F CX1G CX1H HX1V    750.0 0    60.00 ! Nobs =    1 ... Value =
59.98
 DIHEdral HX1R CX1G CX1H HX1T    750.0 0   -60.00 ! Nobs =    1 ... Value =
-61.34
 DIHEdral HX1R CX1G CX1H HX1U    750.0 0    60.00 ! Nobs =    1 ... Value =
58.66
 DIHEdral HX1R CX1G CX1H HX1V    750.0 0   180.00 ! Nobs =    1 ... Value =
178.63
 DIHEdral HX1S CX1G CX1H HX1T    750.0 0    60.00 ! Nobs =    1 ... Value =
61.37
 DIHEdral HX1S CX1G CX1H HX1U    750.0 0   180.00 ! Nobs =    1 ... Value =
-178.63
 DIHEdral HX1S CX1G CX1H HX1V    750.0 0   -60.00 ! Nobs =    1 ... Value =
-58.66
 DIHEdral CX1  OX14 PX14 OX1E    750.0 0    90.00 ! Nobs =    1 ... Value =
83.90
 DIHEdral CX9  OX1F PX14 OX1D    750.0 0     0.00 ! Nobs =    1 ... Value =
-6.97

 { edit if necessary }
! >>> NOTE - unusual value for following improper :    43.99 reset to +35.0
 IMPRoper CX1  HX2  HX3  CX4     750.0 0   40.000 ! Nobs =    1 ... Value =
```

```
43.987
 IMPRoper CX4  CX1  HX5  CX6     750.0 0   35.000 ! Nobs =    1 ... Value =
38.547
 IMPRoper CX6  CX4  HX7  HX8     750.0 0   35.000 ! Nobs =    1 ... Value =
33.155
! >>> NOTE - unusual value for following improper :    46.75 reset to +35.0
 IMPRoper CX9  HX10 HX11 CX12    750.0 0   40.000 ! Nobs =    1 ... Value =
46.745
 IMPRoper CX12 CX9  HX13 HX14    750.0 0   35.000 ! Nobs =    1 ... Value =
33.197
 IMPRoper CX15 HX16 HX17 HX18    750.0 0   35.000 ! Nobs =    1 ... Value =
35.317
 IMPRoper CX19 HX20 HX21 HX22    750.0 0   35.000 ! Nobs =    1 ... Value =
35.312
 IMPRoper CX23 HX24 HX25 HX26    750.0 0   35.000 ! Nobs =    1 ... Value =
35.328
 IMPRoper CX27 CX28 OX1A OX1B    750.0 0    0.000 ! Nobs =    1 ... Value =
0.877
 IMPRoper CX28 CX27 HX29 HX30    750.0 0   35.000 ! Nobs =    1 ... Value =
32.974
 IMPRoper CX31 CX28 HX32 HX33    750.0 0   35.000 ! Nobs =    1 ... Value =
32.923
 IMPRoper CX34 CX31 HX35 HX36    750.0 0   35.000 ! Nobs =    1 ... Value =
33.221
 IMPRoper CX37 CX34 HX38 HX39    750.0 0   35.000 ! Nobs =    1 ... Value =
32.930
 IMPRoper CX40 CX37 HX41 HX42    750.0 0   35.000 ! Nobs =    1 ... Value =
33.436
 IMPRoper CX43 CX40 HX44 HX45    750.0 0   35.000 ! Nobs =    1 ... Value =
33.410
 IMPRoper CX46 CX43 HX47 HX48    750.0 0   35.000 ! Nobs =    1 ... Value =
33.308
 IMPRoper CX49 CX46 HX50 HX51    750.0 0   35.000 ! Nobs =    1 ... Value =
33.449
 IMPRoper CX52 CX49 HX53 HX54    750.0 0   35.000 ! Nobs =    1 ... Value =
33.426
 IMPRoper CX55 CX52 HX56 HX57    750.0 0   35.000 ! Nobs =    1 ... Value =
33.027
 IMPRoper CX58 CX55 HX59 HX60    750.0 0   35.000 ! Nobs =    1 ... Value =
32.900
 IMPRoper CX61 CX58 HX62 HX63    750.0 0   35.000 ! Nobs =    1 ... Value =
32.951
 IMPRoper CX64 CX61 HX65 HX66    750.0 0   35.000 ! Nobs =    1 ... Value =
33.332
 IMPRoper CX67 CX64 HX68 HX69    750.0 0   35.000 ! Nobs =    1 ... Value =
33.403
 IMPRoper CX70 CX67 HX71 HX72    750.0 0   35.000 ! Nobs =    1 ... Value =
33.089
 IMPRoper CX73 CX70 HX74 HX75    750.0 0   35.000 ! Nobs =    1 ... Value =
33.069
 IMPRoper CX76 CX73 HX77 HX78    750.0 0  -35.000 ! Nobs =    1 ... Value =
-33.277
 IMPRoper CX80 CX81 OX13 OX1C    750.0 0    0.000 ! Nobs =    1 ... Value =
-0.273
 IMPRoper CX81 CX80 HX82 HX83    750.0 0   35.000 ! Nobs =    1 ... Value =
33.075
 IMPRoper CX84 CX81 HX85 HX86    750.0 0   35.000 ! Nobs =    1 ... Value =
33.254
 IMPRoper CX87 CX84 HX88 HX89    750.0 0   35.000 ! Nobs =    1 ... Value =
33.061
 IMPRoper CX90 CX87 HX91 HX92    750.0 0   35.000 ! Nobs =    1 ... Value =
```

```
33.383
 IMPRoper CX93 CX90 HX94 HX95    750.0 0   35.000 ! Nobs =    1 ... Value =
32.974
 IMPRoper CX96 CX93 HX97 HX98    750.0 0   35.000 ! Nobs =    1 ... Value =
33.332
 IMPRoper CX99 CX96 HX1A HX1B    750.0 0   35.000 ! Nobs =    1 ... Value =
33.230
 IMPRoper CX10 CX99 HX1C HX1D    750.0 0   35.000 ! Nobs =    1 ... Value =
33.488
 IMPRoper CX1A CX10 HX1E HX1F    750.0 0   35.000 ! Nobs =    1 ... Value =
33.098
 IMPRoper CX1B CX1A HX1G HX1H    750.0 0   35.000 ! Nobs =    1 ... Value =
33.363
 IMPRoper CX11 CX1B HX1I HX1J    750.0 0   35.000 ! Nobs =    1 ... Value =
32.977
 IMPRoper CX1C CX11 HX1K HX1L    750.0 0   35.000 ! Nobs =    1 ... Value =
33.568
 IMPRoper CX1D CX1C HX1M HX1N    750.0 0   35.000 ! Nobs =    1 ... Value =
33.221
 IMPRoper CX1E CX1D HX12 HX1O    750.0 0   35.000 ! Nobs =    1 ... Value =
33.294
 IMPRoper CX1F CX1E HX1P HX1Q    750.0 0   35.000 ! Nobs =    1 ... Value =
33.035
 IMPRoper CX1G CX1F HX1R HX1S    750.0 0   35.000 ! Nobs =    1 ... Value =
33.444
 IMPRoper CX1H CX1G HX1T HX1U    750.0 0  -35.000 ! Nobs =    1 ... Value =
-33.329
 IMPRoper NX13 CX12 CX15 CX19    750.0 0  -35.000 ! Nobs =    1 ... Value =
-33.140
 IMPRoper PX14 OX1D OX1E OX14    750.0 0   35.000 ! Nobs =    1 ... Value =
34.950

 { edit if necessary }
 NONBonded CX1  0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX2  0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX3  0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX4  0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX5  0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX6  0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX7  0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX8  0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX9  0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX10 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX11 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX12 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX13 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX14 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX15 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX16 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX17 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX18 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX19 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX20 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX21 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX22 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX23 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX24 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX25 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX26 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX27 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded CX28 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
```

```
NONBonded HX29 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX30 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX31 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX32 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX33 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX34 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX35 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX36 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX37 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX38 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX39 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX40 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX41 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX42 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX43 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX44 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX45 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX46 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX47 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX48 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX49 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX50 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX51 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX52 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX53 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX54 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX55 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX56 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX57 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX58 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX59 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX60 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX61 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX62 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX63 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX64 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX65 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX66 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX67 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX68 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX69 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX70 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX71 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX72 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX73 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX74 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX75 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX76 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX77 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX78 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX79 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX80 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded CX81 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX82 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX83 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX84 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX85 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX86 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded CX87 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
NONBonded HX88 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
NONBonded HX89 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
```

```
 NONBonded CX90 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX91 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX92 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX93 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX94 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX95 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX96 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX97 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX98 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX99 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX1A 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX1B 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX10 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX1C 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX1D 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX1A 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX1E 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX1F 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX1B 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX1G 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX1H 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX11 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX1I 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX1J 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX1C 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX1K 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX1L 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX1D 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX1M 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX1N 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX1E 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX12 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX1O 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX1F 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX1P 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX1Q 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX1G 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX1R 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX1S 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded CX1H 0.1200  3.7418    0.1000  3.3854 ! assuming Carbon
 NONBonded HX1T 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX1U 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded HX1V 0.0498  1.4254    0.0498  1.4254 ! assuming Hydrogen
 NONBonded NX13 0.2384  2.8509    0.2384  2.8509 ! assuming Nitrogen
 NONBonded OX13 0.1591  2.8509    0.1591  2.8509 ! assuming Oxygen
 NONBonded OX1A 0.1591  2.8509    0.1591  2.8509 ! assuming Oxygen
 NONBonded OX1B 0.1591  2.8509    0.1591  2.8509 ! assuming Oxygen
 NONBonded OX1C 0.1591  2.8509    0.1591  2.8509 ! assuming Oxygen
 NONBonded OX1D 0.1591  2.8509    0.1591  2.8509 ! assuming Oxygen
 NONBonded OX1E 0.1591  2.8509    0.1591  2.8509 ! assuming Oxygen
 NONBonded OX14 0.1591  2.8509    0.1591  2.8509 ! assuming Oxygen
 NONBonded OX1F 0.1591  2.8509    0.1591  2.8509 ! assuming Oxygen
 NONBonded PX14 0.5849  3.3854    0.5849  3.3854 ! assuming Phosphorous

 set echo=true end



topallhdg.hs
remark  file topallhdg.pro
```

```
remark   geometric energy function topology for distance geometry and
remark   simulated annealing.
remark
remark   history:
remark
remark     XPLOR topology file TOPALLHSA.PRO, all hydrogens,
remark     for simulated annealing, to be used with PARALLHSA.PRO
remark     based on TOPALLH6.PRO.
remark     internal coordinates from TOPH19.PRO.

! all dihedrals defining planarity have been converted to impropers,
! the only dihedrals left are around rotatable bonds.
! some additional impropers were included in the rings to define planarity
! better. patches are included to define chirality at stereospecifically
! assigned prochiral centres and convert from trans to cis peptide bond.
! modifications by M. Nilges and P. Kraulis.
! added stereospecific impropers for all pro-chiral centers (ATB)


set message off echo off end

autogenerate
  angles=true
  dihedrals=false
end

mass H    1.008
mass HC   1.008
mass HA   1.008
mass C   12.011
mass CT  12.011
mass CX  12.011
mass CW  12.011
mass CN  12.011
mass CA  12.011
mass CB  12.011
mass CC  12.011
mass CV  12.011
mass CR  12.011
mass CP  12.011
mass N   14.007
mass NA  14.007
mass NB  14.007
mass NH1 14.007
mass NH2 14.007
mass NH3 14.007
mass NC2 14.007
mass O   15.999
mass OC  15.999
mass OH  15.999
mass S   32.060


residue ALA
  group
    atom N   type=NH1 charge=-0.36 end
    atom HN  type=H   charge= 0.26 end
    atom CA  type=CT  charge= 0.00 end
    atom HA  type=HA  charge= 0.10 end
    atom CB  type=CT  charge=-0.30 end
    atom HB1 type=HA  charge= 0.10 end
```

```
    atom HB2 type=HA  charge= 0.10 end
    atom HB3 type=HA  charge= 0.10 end
    atom C   type=C   charge= 0.48 end
    atom O   type=O   charge=-0.48 end

  bond N  HN
  bond N  CA    bond CA  HA
  bond CA  CB   bond CB  HB1   bond CB  HB2     bond CB  HB3
  bond CA  C
  bond C   O

  improper HA  N   C   CB  !stereo CA
  improper HB1 HB2 CA HB3  !stereo CB

  ic N C *CA CB  0.0 0.0  120.0  0.0 0.0
end


residue ARG
  group
    atom N    type=NH1  charge=-0.36 end
    atom HN   type=H    charge= 0.26 end
    atom CA   type=CT   charge= 0.00 end
    atom HA   type=HA   charge= 0.10 end
    atom CB   type=CT   charge=-0.20 end
    atom HB1  type=HA   charge= 0.10 end
    atom HB2  type=HA   charge= 0.10 end
    atom CG   type=CT   charge=-0.20 end
    atom HG1  type=HA   charge= 0.10 end
    atom HG2  type=HA   charge= 0.10 end
    atom CD   type=CT   charge=-0.10 end
    atom HD1  type=HA   charge= 0.15 end
    atom HD2  type=HA   charge= 0.15 end
    atom NE   type=NH1  charge=-0.60 end
    atom HE   type=H    charge= 0.40 end
    atom CZ   type=C    charge= 0.60 end
    atom NH1  type=NC2  charge=-0.60 end
    atom HH11 type=HC   charge= 0.40 end
    atom HH12 type=HC   charge= 0.40 end
    atom NH2   type=NC2 charge=-0.60 end
    atom HH21  type=HC  charge= 0.40 end
    atom HH22  type=HC  charge= 0.40 end
    atom C     type=C   charge= 0.48 end
    atom O     type=O   charge=-0.48 end

  bond N  HN
  bond N  CA     bond CA  HA
  bond CA CB     bond CB  HB1     bond CB  HB2
  bond CB CG     bond CG  HG1     bond CG  HG2
  bond CG CD     bond CD  HD1     bond CD  HD2
  bond CD NE     bond NE  HE
  bond NE CZ
  bond CZ NH1    bond NH1 HH11    bond NH1 HH12
  bond CZ NH2    bond NH2 HH21    bond NH2 HH22
  bond CA C
  bond C  O

  improper HA  N  C    CB  !stereo CA
  improper NE  CD CZ   HE
  improper CZ  NE NH1  NH2
  improper NH1 CZ HH11 HH12
```

```
  improper NH2 CZ HH21 HH22
  improper NE  CZ NH1  HH11
  improper NE  CZ NH2  HH21
!  improper CZ  NH1 HE NE  ! planar HE, CZ
  improper HB1 HB2 CA CG  !stereo CB
  improper HG1 HG2 CB CD  !stereo CG
  improper HD1 HD2 CG NE  !stereo CD

  dihedral CG  CB  CA  N
  dihedral CD  CG  CB  CA
  dihedral NE  CD  CG  CB
  dihedral CZ  NE  CD  CG

  ic N   C  *CA CB   0.0 0.0  120.0  0.0 0.0
  ic N   CA CB  CG   0.0 0.0  180.0  0.0 0.0
  ic CA  CB CG  CD   0.0 0.0  180.0  0.0 0.0
  ic CB  CG CD  NE   0.0 0.0  180.0  0.0 0.0
  ic CG  CD NE  CZ   0.0 0.0  180.0  0.0 0.0
  ic CD  NE CZ  NH1  0.0 0.0  180.0  0.0 0.0
  ic NH1 NE *CZ NH2  0.0 0.0  180.0  0.0 0.0
  ic CD  CZ *NE HE   0.0 0.0  180.0  0.0 0.0
end

residue ASN
  group
    atom N    type=NH1 charge=-0.36 end
    atom HN   type=H   charge= 0.26 end
    atom CA   type=CT  charge= 0.00 end
    atom HA   type=HA  charge= 0.10 end
    atom CB   type=CT  charge=-0.20 end
    atom HB1  type=HA  charge= 0.10 end
    atom HB2  type=HA  charge= 0.10 end
    atom CG   type=C   charge= 0.48 end
    atom OD1  type=O   charge=-0.48 end
    atom ND2  type=NH2 charge=-0.52 end
    atom HD21 type=H   charge= 0.26 end
    atom HD22 type=H   charge= 0.26 end
    atom C    type=C   charge= 0.48 end
    atom O    type=O   charge=-0.48 end

  bond N  HN
  bond N  CA     bond CA  HA
  bond CA CB     bond CB  HB1     bond CB  HB2
  bond CB CG
  bond CG OD1
  bond CG ND2    bond ND2 HD21    bond ND2 HD22
  bond CA C
  bond C  O

  improper HA  N  C    CB  !stereo CA
  improper CG  CB OD1  ND2
  improper ND2 CG HD21 HD22
  improper CB  CG ND2  HD21
  improper HB1 HB2 CA CG  !stereo CB

  dihedral CG  CB  CA  N
  dihedral OD1 CG  CB  CA

  ic N   C  *CA CB   0.0 0.0  120.0  0.0 0.0
  ic N   CA CB  CG   0.0 0.0  180.0  0.0 0.0
  ic CA  CB CG  OD1  0.0 0.0  180.0  0.0 0.0
```

```
  ic OD1 CB *CG ND2  0.0 0.0  180.0  0.0 0.0
end


residue ASP
  group
    atom N   type=NH1 charge=-0.36 end
    atom HN  type=H   charge= 0.26 end
    atom CA  type=CT  charge= 0.00 end
    atom HA  type=HA  charge= 0.10 end
    atom CB  type=CT  charge=-0.45 end
    atom HB1 type=HA  charge= 0.10 end
    atom HB2 type=HA  charge= 0.10 end
    atom CG  type=C   charge= 0.49 end
    atom OD1 type=OC  charge=-0.62 end
    atom OD2 type=OC  charge=-0.62 end
    atom C   type=C   charge= 0.48 end
    atom O   type=O   charge=-0.48 end

  bond N  HN
  bond N  CA     bond CA HA
  bond CA CB     bond CB HB1     bond CB HB2
  bond CB CG
  bond CG OD1
  bond CG OD2
  bond CA C
  bond C  O

  improper HA N  C   CB   !stereo CA
  improper CG CB OD1 OD2
  improper HB1 HB2 CA CG  !stereo CB

  dihedral CG  CB  CA  N
  dihedral OD1 CG  CB  CA

  ic N   C  *CA CB   0.0 0.0  120.0  0.0 0.0
  ic N   CA CB  CG   0.0 0.0  180.0  0.0 0.0
  ic CA  CB CG  OD1  0.0 0.0  180.0  0.0 0.0
  ic OD1 CB *CG OD2  0.0 0.0  180.0  0.0 0.0
end


residue CYS
  group
    atom N   type=NH1 charge=-0.36 end
    atom HN  type=H   charge= 0.26 end
    atom CA  type=CT  charge= 0.00 end
    atom HA  type=HA  charge= 0.10 end
    atom CB  type=CT  charge=-0.20 end
    atom HB1 type=HA  charge= 0.10 end
    atom HB2 type=HA  charge= 0.10 end
    atom SG  type=S   charge=-0.05 end
    atom HG  type=H   charge= 0.05 end
    atom C   type=C   charge= 0.48 end
    atom O   type=O   charge=-0.48 end

  bond N  HN
  bond N  CA     bond CA HA
  bond CA CB     bond CB HB1     bond CB HB2
  bond CB SG     bond SG HG
  bond CA C
```

```
  bond C  O

  improper HA N C CB   !stereo CA
  improper HB1 HB2 CA SG  !stereo CB

  dihedral SG  CB  CA  N

  ic N C  *CA CB  0.0 0.0  120.0  0.0 0.0
  ic N CA CB  SG  0.0 0.0  180.0  0.0 0.0
end


residue GLN
  group
    atom N    type=NH1 charge=-0.36 end
    atom HN   type=H   charge= 0.26 end
    atom CA   type=CT  charge= 0.00 end
    atom HA   type=HA  charge= 0.10 end
    atom CB   type=CT  charge=-0.20 end
    atom HB1  type=HA  charge= 0.10 end
    atom HB2  type=HA  charge= 0.10 end
    atom CG   type=CT  charge=-0.20 end
    atom HG1  type=HA  charge= 0.10 end
    atom HG2  type=HA  charge= 0.10 end
    atom CD   type=C   charge= 0.48 end
    atom OE1  type=O   charge=-0.48 end
    atom NE2  type=NH2 charge=-0.52 end
    atom HE21 type=H   charge= 0.26 end
    atom HE22 type=H   charge= 0.26 end
    atom C    type=C   charge= 0.48 end
    atom O    type=O   charge=-0.48 end

  bond N  HN
  bond N  CA     bond CA  HA
  bond CA CB     bond CB  HB1     bond CB  HB2
  bond CB CG     bond CG  HG1     bond CG  HG2
  bond CG CD
  bond CD OE1
  bond CD NE2    bond NE2 HE21    bond NE2 HE22
  bond CA C
  bond C  O

  improper HA  N  C    CB  !stereo CA
  improper CD  CG OE1  NE2
  improper NE2 CD HE21 HE22
  improper CG  CD NE2  HE21
  improper HB1 HB2 CA CG  !stereo CB
  improper HG1 HG2 CB CD  !stereo CG

  dihedral CG  CB  CA  N
  dihedral CD  CG  CB  CA
  dihedral OE1 CD  CG  CB

  ic N   C  *CA CB   0.0 0.0  120.0  0.0 0.0
  ic N   CA CB  CG   0.0 0.0  180.0  0.0 0.0
  ic CA  CB CG  CD   0.0 0.0  180.0  0.0 0.0
  ic CB  CG CD  OE1  0.0 0.0  180.0  0.0 0.0
  ic OE1 CG *CD NE2  0.0 0.0  180.0  0.0 0.0
end
```

```
residue GLU
  group
    atom N   type=NH1 charge=-0.36 end
    atom HN  type=H   charge= 0.26 end
    atom CA  type=CT  charge= 0.00 end
    atom HA  type=HA  charge= 0.10 end
    atom CB  type=CT  charge=-0.20 end
    atom HB1 type=HA  charge= 0.10 end
    atom HB2 type=HA  charge= 0.10 end
    atom CG  type=CT  charge=-0.45 end
    atom HG1 type=HA  charge= 0.10 end
    atom HG2 type=HA  charge= 0.10 end
    atom CD  type=C   charge= 0.49 end
    atom OE1 type=OC  charge=-0.62 end
    atom OE2 type=OC  charge=-0.62 end
    atom C   type=C   charge= 0.48 end
    atom O   type=O   charge=-0.48 end

  bond N  HN
  bond N  CA     bond CA HA
  bond CA CB     bond CB HB1     bond CB HB2
  bond CB CG     bond CG HG1     bond CG HG2
  bond CG CD
  bond CD OE1
  bond CD OE2
  bond CA C
  bond C  O

  improper HA N  C   CB    !stereo CA
  improper CD CG OE1 OE2
  improper HB1 HB2 CA CG  !stereo CB
  improper HG1 HG2 CB CD  !stereo CG

  dihedral CG  CB  CA  N
  dihedral CD  CG  CB  CA
  dihedral OE1 CD  CG  CB

  ic N   C  *CA CB   0.0 0.0  120.0  0.0 0.0
  ic N   CA CB  CG   0.0 0.0  180.0  0.0 0.0
  ic CA  CB CG  CD   0.0 0.0  180.0  0.0 0.0
  ic CB  CG CD  OE1  0.0 0.0  180.0  0.0 0.0
  ic OE1 CG *CD OE2  0.0 0.0  180.0  0.0 0.0
end


residue GLY
  group
    atom N   type=NH1 charge=-0.36 end
    atom HN  type=H   charge= 0.26 end
    atom CA  type=CT  charge=-0.10 end
    atom HA1 type=HA  charge= 0.10 end
    atom HA2 type=HA  charge= 0.10 end
    atom C   type=C   charge= 0.48 end
    atom O   type=O   charge=-0.48 end

  bond N  HN
  bond N  CA     bond CA HA1     bond CA HA2
  bond CA C
  bond C  O

  improper HA1 HA2 N C  !stereo CA
```

```
end

residue HIS
  group
    atom N   type=NH1 charge=-0.36 end
    atom HN  type=H   charge= 0.26 end
    atom CA  type=CT  charge= 0.00 end
    atom HA  type=HA  charge= 0.10 end
    atom CB  type=CT  charge=-0.20 end
    atom HB1 type=HA  charge= 0.10 end
    atom HB2 type=HA  charge= 0.10 end
    atom CG  type=CC  charge= 0.05 end
    atom ND1 type=NA  charge=-0.40 end
    atom HD1 type=H   charge= 0.40 end
    atom CD2 type=CV  charge=-0.14 end
    atom HD2 type=HA  charge= 0.14 end
    atom CE1 type=CR  charge=-0.14 end
    atom HE1 type=HA  charge= 0.14 end
    atom NE2 type=NB  charge=-0.05 end
    atom C   type=C   charge= 0.48 end
    atom O   type=O   charge=-0.48 end

  bond N   HN
  bond N   CA     bond CA  HA
  bond CA  CB     bond CB  HB1     bond CB  HB2
  bond CB  CG
  bond CG  ND1    bond ND1 HD1
  bond ND1 CE1    bond CE1 HE1
  bond CG  CD2    bond CD2 HD2
  bond CD2 NE2
  bond CE1 NE2
  bond CA  C
  bond C   O

  improper HA  N   C   CB  !stereo CA
  improper CG  CB  ND1 CD2
  improper ND1 CE1 CG  HD1
  improper CD2 NE2 CG  HD2
  improper CE1 ND1 NE2 HE1
  improper CG  ND1 CE1 NE2
  improper ND1 CE1 NE2 CD2
  improper CE1 NE2 CD2 CG
  improper NE2 CD2 CG  ND1
  improper CD2 CG  ND1 CE1
  improper HB1 HB2 CA CG  !stereo CB

  dihedral CG  CB  CA  N
  dihedral ND1 CG  CB  CA

  ic N   C  *CA CB   0.0 0.0  120.0  0.0  0.0
  ic N   CA CB  CG   0.0 0.0  180.0  0.0  0.0
  ic CA  CB CG  CD2  0.0 0.0   90.0  0.0  0.0
  ic CD2 CB *CG ND1  0.0 0.0  180.0  0.0  0.0
  ic CD2 CG ND1 CE1  0.0 0.0    0.0  0.0  0.0
  ic ND1 CG CD2 NE2  0.0 0.0    0.0  0.0  0.0
end

residue ILE
  group
```

```
    atom N    type=NH1 charge=-0.36 end
    atom HN   type=H   charge= 0.26 end
    atom CA   type=CT  charge= 0.00 end
    atom HA   type=HA  charge= 0.10 end
    atom CB   type=CT  charge=-0.10 end
    atom HB   type=HA  charge= 0.10 end
    atom CG1  type=CT  charge=-0.20 end
    atom HG11 type=HA  charge= 0.10 excl = (HG21 HG22 HG23 HD11 HD12 HD13)
end
    atom HG12 type=HA  charge= 0.10 excl = (HG21 HG22 HG23 HD11 HD12 HD13)
end
    atom CG2  type=CT  charge=-0.30 end
    atom HG21 type=HA  charge= 0.10 excl = (HG11 HG12 HD11 HD12 HD13) end
    atom HG22 type=HA  charge= 0.10 excl = (HG11 HG12 HD11 HD12 HD13) end
    atom HG23 type=HA  charge= 0.10 excl = (HG11 HG12 HD11 HD12 HD13) end
    atom CD1  type=CT  charge=-0.30 end
    atom HD11 type=HA  charge= 0.10 excl = (HG21 HG22 HG23 HG11 HG12) end
    atom HD12 type=HA  charge= 0.10 excl = (HG21 HG22 HG23 HG11 HG12) end
    atom HD13 type=HA  charge= 0.10 excl = (HG21 HG22 HG23 HG11 HG12) end
    atom C    type=C   charge= 0.48 end
    atom O    type=O   charge=-0.48 end

  bond N   HN
  bond N   CA     bond CA  HA
  bond CA  CB     bond CB  HB
  bond CB  CG1    bond CG1 HG11    bond CG1 HG12
  bond CB  CG2    bond CG2 HG21    bond CG2 HG22    bond CG2 HG23
  bond CG1 CD1    bond CD1 HD11    bond CD1 HD12    bond CD1 HD13
  bond CA  C
  bond C   O

  improper HA N  C   CB   !stereo CA
  improper CA HB CG2 CG1  !stereo CB

  improper HG11 HG12 CB CD1  !stereo CG1
  improper HG21 HG22 CB HG23  !stereo CG2
  improper HD11 HD12 CG1 HD13  !stereo CD1

  dihedral CG1 CB  CA  N
  dihedral CD1 CG1 CB  CA

  ic N  C  *CA CB   0.0 0.0  120.0  0.0 0.0
  ic N  CA CB  CG1  0.0 0.0  180.0  0.0 0.0
  ic N  CA CB  CG2  0.0 0.0   60.0  0.0 0.0
  ic CA CB CG1 CD1   0.0 0.0  180.0  0.0 0.0
end


residue LEU
  group
    atom N    type=NH1 charge=-0.36 end
    atom HN   type=H   charge= 0.26 end
    atom CA   type=CT  charge= 0.00 end
    atom HA   type=HA  charge= 0.10 end
    atom CB   type=CT  charge=-0.20 end
    atom HB1  type=HA  charge= 0.10 end
    atom HB2  type=HA  charge= 0.10 end
    atom CG   type=CT  charge=-0.10 end
    atom HG   type=HA  charge= 0.10 end
    atom CD1  type=CT  charge=-0.30 end
    atom HD11 type=HA  charge= 0.10 excl = (HD21 HD22 HD23 HG) end
```

```
    atom HD12 type=HA  charge= 0.10 excl = (HD21 HD22 HD23 HG) end
    atom HD13 type=HA  charge= 0.10 excl = (HD21 HD22 HD23 HG) end
    atom CD2  type=CT  charge=-0.30 end
    atom HD21 type=HA  charge= 0.10 excl = (HD11 HD12 HD13 HG) end
    atom HD22 type=HA  charge= 0.10 excl = (HD11 HD12 HD13 HG) end
    atom HD23 type=HA  charge= 0.10 excl = (HD11 HD12 HD13 HG) end
    atom C    type=C   charge= 0.48 end
    atom O    type=O   charge=-0.48 end

  bond N   HN
  bond N   CA     bond CA  HA
  bond CA  CB     bond CB  HB1     bond CB  HB2
  bond CB  CG     bond CG  HG
  bond CG  CD1    bond CD1 HD11    bond CD1 HD12    bond CD1 HD13
  bond CG  CD2    bond CD2 HD21    bond CD2 HD22    bond CD2 HD23
  bond CA  C
  bond C   O

  improper HA   N    C   CB
  improper HG   CB   CD1 CD2   !stereo CG
  improper HB1 HB2 CA CG       !stereo CB
  improper HD11 HD12 CG HD13   !stereo CD1
  improper HD21 HD22 CG HD23   !stereo CD2

  dihedral CG  CB  CA  N
  dihedral CD1 CG  CB  CA

  ic N  C  *CA CB   0.0 0.0  120.0  0.0 0.0
  ic N  CA CB  CG   0.0 0.0  180.0  0.0 0.0
  ic CA CB CG  CD1  0.0 0.0  180.0  0.0 0.0
  ic CA CB CG  CD2  0.0 0.0  -60.0  0.0 0.0
end


residue LYS
  group
    atom N   type=NH1 charge=-0.360 end
    atom HN  type=H   charge= 0.260 end
    atom CA  type=CT  charge= 0.000 end
    atom HA  type=HA  charge= 0.100 end
    atom CB  type=CT  charge=-0.200 end
    atom HB1 type=HA  charge= 0.100 end
    atom HB2 type=HA  charge= 0.100 end
    atom CG  type=CT  charge=-0.200 end
    atom HG1 type=HA  charge= 0.100 end
    atom HG2 type=HA  charge= 0.100 end
    atom CD  type=CT  charge=-0.200 end
    atom HD1 type=HA  charge= 0.100 end
    atom HD2 type=HA  charge= 0.100 end
    atom CE  type=CT  charge= 0.305 end
    atom HE1 type=HA  charge= 0.100 end
    atom HE2 type=HA  charge= 0.100 end
    atom NZ  type=NH3 charge=-0.810 end
    atom HZ1 type=HC  charge= 0.435 end
    atom HZ2 type=HC  charge= 0.435 end
    atom HZ3 type=HC  charge= 0.435 end
    atom C   type=C   charge= 0.480 end
    atom O   type=O   charge=-0.480 end

  bond N  HN
  bond N  CA     bond CA HA
```

```
  bond CA CB     bond CB HB1     bond CB HB2
  bond CB CG     bond CG HG1     bond CG HG2
  bond CG CD     bond CD HD1     bond CD HD2
  bond CD CE     bond CE HE1     bond CE HE2
  bond CE NZ     bond NZ HZ1     bond NZ HZ2     bond NZ HZ3
  bond CA C
  bond C  O

  improper HA N C CB      !stereo CA
  improper HB1 HB2 CA CG  !stereo CB
  improper HG1 HG2 CB CD  !stereo CG
  improper HD1 HD2 CG CE  !stereo CD
  improper HE1 HE2 CD NZ  !stereo CE
  improper HZ1 HZ2 CE HZ3 !stereo NZ

  dihedral CG  CB  CA  N
  dihedral CD  CG  CB  CA
  dihedral CE  CD  CG  CB
  dihedral NZ  CE  CD  CG

  ic N  C  *CA CB  0.0 0.0  120.0  0.0 0.0
  ic N  CA CB  CG  0.0 0.0  180.0  0.0 0.0
  ic CA CB CG  CD  0.0 0.0  180.0  0.0 0.0
  ic CB CG CD  CE  0.0 0.0  180.0  0.0 0.0
  ic CG CD CE  NZ  0.0 0.0  180.0  0.0 0.0
end

residue MET
  group
    atom N   type=NH1 charge=-0.360 end
    atom HN  type=H   charge= 0.260 end
    atom CA  type=CT  charge= 0.000 end
    atom HA  type=HA  charge= 0.100 end
    atom CB  type=CT  charge=-0.200 end
    atom HB1 type=HA  charge= 0.100 end
    atom HB2 type=HA  charge= 0.100 end
    atom CG  type=CT  charge=-0.115 end
    atom HG1 type=HA  charge= 0.100 end
    atom HG2 type=HA  charge= 0.100 end
    atom SD  type=S   charge=-0.170 end
    atom CE  type=CT  charge=-0.215 end
    atom HE1 type=HA  charge= 0.100 end
    atom HE2 type=HA  charge= 0.100 end
    atom HE3 type=HA  charge= 0.100 end
    atom C   type=C   charge= 0.480 end
    atom O   type=O   charge=-0.480 end

  bond N  HN
  bond N  CA     bond CA HA
  bond CA CB     bond CB HB1     bond CB HB2
  bond CB CG     bond CG HG1     bond CG HG2
  bond CG SD
  bond SD CE     bond CE HE1     bond CE HE2     bond CE HE3
  bond CA C
  bond C  O

  improper HA N C CB      !stereo CA
  improper HB1 HB2 CA CG  !stereo CB
  improper HG1 HG2 CB SD  !stereo CG
  improper HE1 HE2 SD HE3 !stereo methyl
```

```
  dihedral CG  CB  CA  N
  dihedral SD  CG  CB  CA
  dihedral CE  SD  CG  CB

  ic N  C  *CA CB  0.0 0.0  120.0  0.0 0.0
  ic N  CA CB  CG  0.0 0.0  180.0  0.0 0.0
  ic CA CB CG  SD  0.0 0.0  180.0  0.0 0.0
  ic CB CG SD  CE  0.0 0.0  180.0  0.0 0.0
end


residue PHE
  group
    atom N   type=NH1 charge=-0.36 end
    atom HN  type=H   charge= 0.26 end
    atom CA  type=CT  charge= 0.00 end
    atom HA  type=HA  charge= 0.10 end
    atom CB  type=CT  charge=-0.16 end
    atom HB1 type=HA  charge= 0.10 end
    atom HB2 type=HA  charge= 0.10 end
    atom CG  type=CA  charge= 0.03 exclude=(CZ) end
    atom CD1 type=CA  charge=-0.16 exclude=(CE2) end
    atom HD1 type=HA  charge= 0.14 end
    atom CD2 type=CA  charge=-0.16 exclude=(CE1) end
    atom HD2 type=HA  charge= 0.14 end
    atom CE1 type=CA  charge=-0.15 exclude=(CD2) end
    atom HE1 type=HA  charge= 0.14 end
    atom CE2 type=CA  charge=-0.15 exclude=(CD1) end
    atom HE2 type=HA  charge= 0.14 end
    atom CZ  type=CA  charge=-0.15 exclude=(CG) end
    atom HZ  type=HA  charge= 0.14 end
    atom C   type=C   charge= 0.48 end
    atom O   type=O   charge=-0.48 end
  bond N   HN
  bond N   CA     bond CA  HA
  bond CA  CB     bond CB  HB1     bond CB  HB2
  bond CB  CG
  bond CG  CD1    bond CD1 HD1
  bond CG  CD2    bond CD2 HD2
  bond CD1 CE1    bond CE1 HE1
  bond CD2 CE2    bond CE2 HE2
  bond CE1 CZ     bond CZ  HZ
  bond CE2 CZ
  bond CA  C
  bond C   O

  improper HA  N   C   CB !stereo CA
  improper HB1 HB2 CA CG  !stereo CB

! Hs and CB around the ring
  improper HD2 CD2 CE2 CZ
  improper HE2 CE2 CZ  CE1
  improper HZ  CZ  CE1 CD1
  improper HE1 CE1 CD1 CG
  improper HD1 CD1 CG  CD2
  improper CB  CG  CD2 CE2

! around the ring
  improper CG  CD1 CE1 CZ
  improper CD1 CE1 CZ  CE2
  improper CE1 CZ  CE2 CD2
```

```
  improper CZ  CE2 CD2 CG
  improper CE2 CD2 CG  CD1
  improper CD2 CG  CD1 CE1

  dihedral CG  CB  CA  N
  dihedral CD1 CG  CB  CA

  ic N   C   *CA CB   0.0 0.0  120.0  0.0 0.0
  ic N   CA  CB  CG   0.0 0.0  180.0  0.0 0.0
  ic CA  CB  CG  CD1  0.0 0.0   90.0  0.0 0.0
  ic CD1 CB  *CG CD2  0.0 0.0  180.0  0.0 0.0
  ic CD1 CG  CD2 CE2  0.0 0.0    0.0  0.0 0.0
  ic CD2 CG  CD1 CE1  0.0 0.0    0.0  0.0 0.0
  ic CG  CD1 CE1 CZ   0.0 0.0    0.0  0.0 0.0
end


residue PRO
  group
    atom N   type=N  charge=-0.36 end
    atom CA  type=CT charge= 0.00 end
    atom HA  type=HA charge= 0.10 end
    atom CB  type=CT charge=-0.20 end
    atom HB1 type=HA charge= 0.10 end
    atom HB2 type=HA charge= 0.10 end
    atom CG  type=CP charge=-0.20 end
    atom HG1 type=HA charge= 0.10 end
    atom HG2 type=HA charge= 0.10 end
    atom CD  type=CP charge= 0.06 end
    atom HD2 type=HA charge= 0.10 end   ! the order of the two h's
    atom HD1 type=HA charge= 0.10 end   ! is inverted for the sake of
    atom C   type=C  charge= 0.48 end   ! hbuild
    atom O   type=O  charge=-0.48 end

  bond N  CA     bond CA HA
  bond CA CB     bond CB HB1     bond CB HB2
  bond CB CG     bond CG HG1     bond CG HG2
  bond CG CD     bond CD HD1     bond CD HD2
  bond CD N
  bond CA C
  bond C  O

  improper HA N C CB      !chiral CA
  improper N CA CB CG     !ring pucker
  improper HB1 HB2 CA CG  !stereo CB
  improper HG1 HG2 CB CD  !stereo CG
  improper HD1 HD2 CG N   !stereo CD

  ic C N  *CA CB  0.0 0.0 -120.0  0.0 0.0
  ic N CA CB  CG  0.0 0.0    0.0  0.0 0.0
end


residue SER
  group
    atom N   type=NH1 charge=-0.36 end
    atom HN  type=H   charge= 0.26 end
    atom CA  type=CT  charge= 0.00 end
    atom HA  type=HA  charge= 0.10 end
    atom CB  type=CT  charge= 0.08 end
    atom HB1 type=HA  charge= 0.10 end
```

```
    atom HB2 type=HA  charge= 0.10 end
    atom OG  type=OH  charge=-0.68 end
    atom HG  type=H   charge= 0.40 end
    atom C   type=C   charge= 0.48 end
    atom O   type=O   charge=-0.48 end

  bond N  HN
  bond N  CA     bond CA HA
  bond CA CB     bond CB HB1     bond CB HB2
  bond CB OG     bond OG HG
  bond O  C
  bond C  CA

  improper HA N C CB      !stereo CA
  improper HB1 HB2 CA OG  !stereo CB

  dihedral OG  CB  CA  N

  ic N C  *CA CB  0.0 0.0  120.0  0.0 0.0
  ic N CA CB  OG  0.0 0.0  180.0  0.0 0.0
end


residue THR
  group
    atom N    type=NH1 charge=-0.36 end
    atom HN   type=H   charge= 0.26 end
    atom CA   type=CT  charge= 0.00 end
    atom HA   type=HA  charge= 0.10 end
    atom CB   type=CT  charge= 0.18 end
    atom HB   type=HA  charge= 0.10 end
    atom OG1  type=OH  charge=-0.68 end
    atom HG1  type=H   charge= 0.40 end
    atom CG2  type=CT  charge=-0.30 end
    atom HG21 type=HA  charge= 0.10 end
    atom HG22 type=HA  charge= 0.10 end
    atom HG23 type=HA  charge= 0.10 end
    atom C    type=C   charge= 0.48 end
    atom O    type=O   charge=-0.48 end

  bond N  HN
  bond N  CA     bond CA HA
  bond CA CB     bond CB HB
  bond CB OG1    bond OG1 HG1
  bond CB CG2    bond CG2 HG21    bond CG2 HG22    bond CG2 HG23
  bond CA C
  bond C  O

  improper HA N  C   CB        !stereo CA
  improper HB CA OG1 CG2       !stereo CB
  improper HG21 HG22 CB HG23  !stereo methyl

  dihedral OG1 CB  CA  N

  ic N C  *CA CB   0.0 0.0  120.0  0.0 0.0
  ic N CA CB  OG1  0.0 0.0  180.0  0.0 0.0
  ic N CA CB  CG2  0.0 0.0   60.0  0.0 0.0
end


residue TRP
```

```
  group
    atom N   type=NH1 charge=-0.36 end
    atom HN  type=H   charge= 0.26 end
    atom CA  type=CT  charge= 0.00 end
    atom HA  type=HA  charge= 0.10 end
    atom CB  type=CT  charge=-0.20 end
    atom HB1 type=HA  charge= 0.10 end
    atom HB2 type=HA  charge= 0.10 end
    atom CG  type=CX  charge=-0.04 end
    atom CD1 type=CW  charge=-0.01 end
    atom HD1 type=HA  charge= 0.14 end
    atom CD2 type=CB  charge=-0.05 exclude=(CH2) end
    atom NE1 type=NA charge=-0.49 end
    atom HE1 type=H   charge= 0.40 end
    atom CE2 type=CN  charge= 0.13 exclude=(CZ3) end
    atom CE3 type=CA  charge=-0.16 exclude=(CZ2) end
    atom HE3 type=HA  charge= 0.14 end
    atom CZ2 type=CA  charge=-0.15 exclude=(CE3) end
    atom HZ2 type=HA  charge= 0.14 end
    atom CZ3 type=CA  charge=-0.15 exclude=(CE2) end
    atom HZ3 type=HA  charge= 0.14 end
    atom CH2 type=CA  charge=-0.18 exclude=(CD2) end
    atom HH2 type=HA  charge= 0.14 end
    atom C   type=C   charge= 0.48 end
    atom O   type=O   charge=-0.48 end

  bond N   HN
  bond N   CA     bond CA  HA
  bond CA  CB     bond CB  HB1     bond CB  HB2
  bond CB  CG
  bond CG  CD1    bond CD1 HD1
  bond CG  CD2
  bond CD1 NE1    bond NE1 HE1
  bond NE1 CE2
  bond CD2 CE2
  bond CD2 CE3    bond CE3 HE3
  bond CE2 CZ2    bond CZ2 HZ2
  bond CE3 CZ3    bond CZ3 HZ3
  bond CZ2 CH2    bond CH2 HH2
  bond CZ3 CH2
  bond CA  C
  bond C   O

! chirality
  improper HA  N   C   CB !stereo CA
  improper HB1 HB2 CA CG  !stereo CB

! around the 6-ring
  improper CD2 CE2 CZ2 CH2
  improper CE2 CZ2 CH2 CZ3
  improper CZ2 CH2 CZ3 CE3
  improper CH2 CZ3 CE3 CD2
  improper CZ3 CE3 CD2 CE2
  improper CE3 CD2 CE2 CZ2

! link 5-ring to 6-ring
  improper CD1 NE1 CE2 CZ2
  improper CD1 CG  CD2 CE3
  improper NE1 CE2 CZ2 CH2
  improper NE1 CE2 CD2 CE3
  improper CG  CD2 CE3 CZ3
```

```
  improper CG  CD2 CE2 CZ2

! 6-ring hydrogens
  improper HZ2 CZ2 CH2 CZ3
  improper HH2 CH2 CZ3 CE3
  improper HZ3 CZ3 CH2 CZ2
  improper HE3 CE3 CZ3 CH2

! 5-ring hydrogens and CB
  improper HE1 NE1 CE2 CD2
  improper HD1 CD1 NE1 CE2
  improper CB  CG  CD2 CE2

  dihedral CG  CB  CA  N
  dihedral CD1 CG  CB  CA

  ic N   C   *CA  CB   0.0 0.0  120.0  0.0 0.0
  ic N   CA  CB   CG   0.0 0.0  180.0  0.0 0.0
  ic CA  CB  CG   CD2  0.0 0.0  180.0  0.0 0.0
  ic CD2 CB  *CG  CD1  0.0 0.0  180.0  0.0 0.0
  ic CD1 CG  CD2  CE2  0.0 0.0    0.0  0.0 0.0
  ic CD2 CG  CD1  NE1  0.0 0.0    0.0  0.0 0.0
  ic CE2 CG  *CD2 CE3  0.0 0.0  180.0  0.0 0.0
  ic CE2 CD2 CE3  CZ3  0.0 0.0    0.0  0.0 0.0
  ic CE3 CD2 CE2  CZ2  0.0 0.0    0.0  0.0 0.0
  ic CD2 CE2 CZ2  CH2  0.0 0.0    0.0  0.0 0.0
end

residue TYR
  group
    atom N   type=NH1 charge=-0.36 end
    atom HN  type=H   charge= 0.26 end
    atom CA  type=CT  charge= 0.00 end
    atom HA  type=HA  charge= 0.10 end
    atom CB  type=CT  charge=-0.20 end
    atom HB1 type=HA  charge= 0.10 end
    atom HB2 type=HA  charge= 0.10 end
    atom CG  type=CA  charge= 0.00 exclude=(CZ) end
    atom CD1 type=CA  charge=-0.14 exclude=(CE2) end
    atom HD1 type=HA  charge= 0.14 end
    atom CD2 type=CA  charge=-0.14 exclude=(CE1) end
    atom HD2 type=HA  charge= 0.14 end
    atom CE1 type=CA  charge=-0.14 exclude=(CD2) end
    atom HE1 type=HA  charge= 0.14 end
    atom CE2 type=CA  charge=-0.14 exclude=(CD1) end
    atom HE2 type=HA  charge= 0.14 end
    atom CZ  type=C   charge= 0.20 exclude=(CG) end
    atom OH  type=OH  charge=-0.60 end
    atom HH  type=H   charge= 0.40 end
    atom C   type=C   charge= 0.48 end
    atom O   type=O   charge=-0.48 end

  bond N   HN
  bond N   CA     bond CA  HA
  bond CA  CB     bond CB  HB1     bond CB  HB2
  bond CB  CG
  bond CG  CD1    bond CD1 HD1
  bond CG  CD2    bond CD2 HD2
  bond CD1 CE1    bond CE1 HE1
  bond CD2 CE2    bond CE2 HE2
  bond CE1 CZ
```

```
  bond CE2 CZ
  bond CZ  OH     bond OH  HH
  bond CA  C
  bond C   O

! chirality
  improper HA  N   C   CB !stereo CA
  improper HB1 HB2 CA CG  !stereo CB

! Hs, OH, and CB around the ring
  improper HD2 CD2 CE2 CZ
  improper HE2 CE2 CZ  CE1
  improper OH  CZ  CE1 CD1
  improper HE1 CE1 CD1 CG
  improper HD1 CD1 CG  CD2
  improper CB  CG  CD2 CE2

! around the ring
  improper CG  CD1 CE1 CZ
  improper CD1 CE1 CZ  CE2
  improper CE1 CZ  CE2 CD2
  improper CZ  CE2 CD2 CG
  improper CE2 CD2 CG  CD1
  improper CD2 CG  CD1 CE1

  dihedral CG  CB  CA  N
  dihedral CD1 CG  CB  CA

  ic N   C   *CA CB   0.0 0.0  120.0  0.0 0.0
  ic N   CA  CB  CG   0.0 0.0  180.0  0.0 0.0
  ic CA  CB  CG  CD1  0.0 0.0   90.0  0.0 0.0
  ic CD1 CB  *CG CD2  0.0 0.0  180.0  0.0 0.0
  ic CD2 CG  CD1 CE1  0.0 0.0    0.0  0.0 0.0
  ic CD1 CG  CD2 CE2  0.0 0.0    0.0  0.0 0.0
  ic CG  CD1 CE1 CZ   0.0 0.0    0.0  0.0 0.0
  ic CE2 CE1 *CZ OH   0.0 0.0  180.0  0.0 0.0
end


residue VAL
  group
    atom N    type=NH1 charge=-0.36 end
    atom HN   type=H   charge= 0.26 end
    atom CA   type=CT  charge= 0.00 end
    atom HA   type=HA  charge= 0.10 end
    atom CB   type=CT  charge=-0.10 end
    atom HB   type=HA  charge= 0.10 end
    atom CG1  type=CT  charge=-0.30 end
    atom HG11 type=HA  charge= 0.10 excl = (HG21 HG22 HG23) end
    atom HG12 type=HA  charge= 0.10 excl = (HG21 HG22 HG23) end
    atom HG13 type=HA  charge= 0.10 excl = (HG21 HG22 HG23) end
    atom CG2  type=CT  charge=-0.30 end
    atom HG21 type=HA  charge= 0.10 excl = (HG11 HG12 HG13) end
    atom HG22 type=HA  charge= 0.10 excl = (HG11 HG12 HG13) end
    atom HG23 type=HA  charge= 0.10 excl = (HG11 HG12 HG13) end
    atom C    type=C   charge= 0.48 end
    atom O    type=O   charge=-0.48 end

  bond N   HN
  bond N   CA     bond CA  HA
  bond CA  CB     bond CB  HB
```

```
  bond CB  CG1    bond CG1 HG11    bond CG1 HG12    bond CG1 HG13
  bond CB  CG2    bond CG2 HG21    bond CG2 HG22    bond CG2 HG23
  bond CA  C
  bond C   O

  improper HA N C CB         !stereo CA
  improper HB   CA   CG1 CG2 !stereo CB
  improper HG11 HG12 CB HG13    !stereo G1
  improper HG21 HG22 CB HG23    !stereo G2

  dihedral CG1 CB  CA  N

  ic N C  *CA CB   0.0 0.0  120.0  0.0 0.0
  ic N CA CB  CG1  0.0 0.0  180.0  0.0 0.0
  ic N CA CB  CG2  0.0 0.0  -60.0  0.0 0.0
end



residue CHEX  !! ADDED BY MN
  group
    atom N   type=NH1 charge=-0.360 end
    atom HN  type=H   charge= 0.260 end
    atom CA  type=CT  charge= 0.000 end
    atom HA  type=HA  charge= 0.100 end
    atom CB  type=CT  charge=-0.200 end
    atom HB1 type=HA  charge= 0.100 end
    atom HB2 type=HA  charge= 0.100 end
    atom CG  type=CT  charge=-0.200 end
    atom HG  type=HA  charge= 0.100 end
    atom CD1  type=CT  charge=-0.200 end
    atom HD11 type=HA  charge= 0.100 end
    atom HD12 type=HA  charge= 0.100 end
    atom CD2  type=CT  charge=-0.200 end
    atom HD21 type=HA  charge= 0.100 end
    atom HD22 type=HA  charge= 0.100 end
    atom CE1  type=CT  charge=-0.200 end
    atom HE11 type=HA  charge= 0.100 end
    atom HE12 type=HA  charge= 0.100 end
    atom CE2  type=CT  charge=-0.200 end
    atom HE21 type=HA  charge= 0.100 end
    atom HE22 type=HA  charge= 0.100 end
    atom CZ  type=CT  charge=-0.200 end
    atom HZ1 type=HA  charge= 0.100 end
    atom HZ2 type=HA  charge= 0.100 end
    atom C   type=C   charge= 0.480 end
    atom O   type=O   charge=-0.480 end

  bond N  HN
  bond N  CA     bond CA HA
  bond CA CB     bond CB HB1     bond CB HB2
  bond CB CG     bond CG CD1     bond CG CD2     bond CG HG
  bond CD1 CE1   bond CD1 HD11    bond CD1 HD12
  bond CD2 CE2   bond CD2 HD21    bond CD2 HD22
  bond CE1 CZ    bond CE1 HE11    bond CE1 HE12
  bond CE2 CZ    bond CE2 HE21    bond CE2 HE22
  bond CZ HZ1    bond CZ  HZ2
  bond CA C
  bond C  O
```

```
  improper HA N C CB          !stereo CA
  improper HB1 HB2 CA CG  !stereo CB
  improper HG CB CD1 CD2      !stereo CG
  improper HD11 HD12 CG CE1      !stereo CD1
  improper HD21 HD22 CG CE2      !stereo CD2
  improper HE11 HE12 CE1 CZ      !stereo CE1
  improper HE11 HE22 CE2 CZ      !stereo CE2
  improper HZ1 HZ2 CE1 CE2  !stereo CZ

  dihedral CG  CB  CA  N
  dihedral CD1  CG  CB  CA

  ic N  C  *CA CB     0.0 0.0   120.0  0.0 0.0
  ic N  CA CB  CG     0.0 0.0   180.0  0.0 0.0
  ic CA CB CG  CD1    0.0 0.0   180.0  0.0 0.0
  ic CB CG CD1 CE1    0.0 0.0   180.0  0.0 0.0
  ic CG CD1 CE1 CZ    0.0 0.0   -60.0  0.0 0.0
  ic CD1 CE1 CZ CE2   0.0 0.0    60.0  0.0 0.0
  ic CE1 CZ CE2 CD2   0.0 0.0   -60.0  0.0 0.0
end




residue ACE
  group
    atom CA  type=CT charge=-0.30 end
    atom HA1 type=HA charge= 0.10 end
    atom HA2 type=HA charge= 0.10 end
    atom HA3 type=HA charge= 0.10 end
    atom C   type=C  charge= 0.48 end
    atom O   type=O  charge=-0.48 end

  bond C  CA     bond CA HA1     bond CA HA2     bond CA HA3
  bond C  O
  improper HA1 HA2 C HA3  !stereo methyl
end



presidue NTER                      ! patch as "NTER - *" to any except PRO
  modify    atom +CA           charge= 0.22 end
  group
    modify    atom +N   type=NH3 charge=-0.10 end
    delete    atom +HN                        end
    add       atom +HT1 type=HC  charge= 0.26 end
    add       atom +HT2 type=HC  charge= 0.26 end
    add       atom +HT3 type=HC  charge= 0.26 end

  add bond +HT1 +N
  add bond +HT2 +N
  add bond +HT3 +N

  add angle +HT1 +N +HT2
  add angle +HT2 +N +HT3
  add angle +HT2 +N +CA
  add angle +HT1 +N +HT3
  add angle +HT1 +N +CA
  add angle +HT3 +N +CA
```

```
  add improper +HT1 +HT2 +CA +HT3  !stereo N ???

end


presidue PROP                          ! N-terminal for PRO: "PROP - PRO"
  modify    atom +CD           charge= 0.10 end
  modify    atom +CA           charge= 0.10 end
  modify    atom +N   type=NH3 charge=-0.02 end
  add       atom +HT1 type=HC  charge= 0.26 end
  add       atom +HT2 type=HC  charge= 0.26 end

  add bond +HT1 +N
  add bond +HT2 +N

  add angle +HT1 +N +HT2
  add angle +HT2 +N +CA
  add angle +HT1 +N +CD
  add angle +HT1 +N +CA
  add angle +CD  +N +HT2
  add improper +HT1 +HT2 +CA +CD  !stereo N
end


presidue CTER               ! C-terminal for all amino acids "* - CTER"
  group
    modify    atom -C           charge= 0.14 end
    delete    atom -O                        end
    add       atom -OT1 type=OC charge=-0.57 end
    add       atom -OT2 type=OC charge=-0.57 end

  add bond -C -OT1
  add bond -C -OT2

  add angle -CA  -C -OT1
  add angle -CA  -C -OT2
  add angle -OT1 -C -OT2

  add improper -C -CA -OT2 -OT1

  add ic -N   -CA -C  -OT2  0.0 0.0  180.0  0.0 0.0
  add ic -OT2 -CA *-C -OT1  0.0 0.0  180.0  0.0 0.0
end


presidue CTN                  ! C-terminal for all, CONH2 at end "* - CTN"
  group
    modify    atom -C           charge= 0.48 end
    modify    atom -O           charge=-0.48 end
    add       atom -NT type=NH2 charge=-0.52 end
    add       atom -H1 type=H   charge= 0.26 end
    add       atom -H2 type=H   charge= 0.26 end

  add bond -C  -NT
  add bond -NT -H1
  add bond -NT -H2

  add angle -CA -C  -NT
  add angle -O  -C  -NT
  add angle -CA -C  -O
  add angle -C  -NT -H1
```

```
  add angle -C  -NT -H2
  add angle -H1 -NT -H2

  add improper -C  -CA -NT -O
  add improper -C  -NT -O  -H1
  add improper -NT -H1 -H2 -C
end


presidue PEPT     ! PEPTide bond link, for all except the  *(-) - (+)PRO
link
                  ! "*(-) - PEPT - (+)*:
  add bond -C +N

  add angle -CA -C +N
  add angle -O  -C +N
  add angle -C  +N +CA
  add angle -C  +N +HN

  add improper -O  -C  +N  +CA                      ! planar -C    fixed for
DG by JK
  add improper +HN +N  -C  -CA                      ! planar +N
  add improper -CA -C  +N  +CA                      ! planar peptide
"

  add ic -C  +CA *+N +H   0.0 0.0  180.0  0.0 0.0  ! planar -C
  add ic -C  +N  +CA +C   0.0 0.0  180.0  0.0 0.0
  add ic -N  -CA -C  +N   0.0 0.0  180.0  0.0 0.0
  add ic -CA -C  +N  +CA  0.0 0.0  180.0  0.0 0.0
  add ic +N  -CA *-C -O   0.0 0.0  180.0  0.0 0.0  ! planar +N
end


presidue PEPP     ! for  ...*(-) - (+)PRO  link, same as PEPT except
                  ! replacement H by CD and improper +N +CA +CD -C
  add bond -C +N

  add angle -CA -C +N
  add angle -O  -C +N
  add angle -C  +N +CA
  add angle -C  +N +CD

  add improper -O  -C  +N  +CA                       ! planar -C
  add improper +CA +N  -C  +CD                       ! planar +N modified
  add improper -CA  -C +N +CA                        ! planar peptide

  add ic -C  +CA *+N +CD  0.0 0.0  180.0  0.0 0.0  ! planar +N
  add ic -C  +N  +CA +C   0.0 0.0  180.0  0.0 0.0
  add ic -N  -CA -C  +N   0.0 0.0  180.0  0.0 0.0
  add ic -CA -C  +N  +CA  0.0 0.0  180.0  0.0 0.0
  add ic +N  -CA *-C -O   0.0 0.0  180.0  0.0 0.0  ! planar -C
end


presidue DISU                ! disulfide bridge  ...CYS - DISU - CYS...
  group
    delete    atom 1HG               end
    modify    atom 1CB  charge= 0.20 end
    modify    atom 1SG  charge=-0.20 end
  group
    delete    atom 2HG               end
```

```
    modify    atom 2CB  charge= 0.20 end
    modify    atom 2SG  charge=-0.20 end

  add bond 1SG 2SG

  add angle 1CB 1SG 2SG
  add angle 1SG 2SG 2CB

  add ic 1CA 1CB 1SG 2SG  0.0 0.0  180.0  0.0 0.0
  add ic 1CB 1SG 2SG 2CB  0.0 0.0  180.0  0.0 0.0
  add ic 1SG 2SG 2CB 2CA  0.0 0.0  180.0  0.0 0.0
end


presidue DISN               ! disulfide bridge  ...CYS - DISU - CYS...
                            ! w/o the actual bond
  group
    delete    atom 1HG               end
    modify    atom 1CB  charge= 0.20 end
    modify    atom 1SG  charge=-0.20 end
  group
    delete    atom 2HG               end
    modify    atom 2CB  charge= 0.20 end
    modify    atom 2SG  charge=-0.20 end
end


presidue LTOD                       ! change from L to D amino acid
  delete improper HA N C CB
  add    improper HA C N CB
end

presidue CISP                       ! change from trans to cis peptide
bond
  delete improper -CA -C  +N  +CA
  add    improper -C  -CA +N  +CA
  delete improper -O  -C  +N  +CA
  add    improper -C  -O  +N  +CA
  delete improper +HN +N  -C  -CA
  add    improper +N  +HN -C  -CA
end

presidue CIPP                       ! change from trans to cis peptide
bond
  delete improper -CA -C  +N  +CA
  add    improper -C  -CA +N  +CA
  delete improper -O  -C  +N  +CA
  add    improper -C  -O  +N  +CA
  delete improper +CA +N  -C  +CD
  add    improper +CA +N  +CD -C
end

presidue HISE     !  change protonation of HIS
                  !  has to be patched as REFErence=NIL=<selection>

  modify atom ND1 type=NA  charge=-0.05 end
  delete atom HD1                       end
  modify atom NE2 type=NB  charge=-0.40 end
  add    atom HE2 type=H   charge= 0.40 end

  add bond HE2 NE2
```

```
  add angle HE2 NE2 CD2
  add angle HE2 NE2 CE1
  add improper NE2 CE1 CD2 HE2

end {HISE}


set echo=true end


parallhdg_min.pn
remark   file parallhdg.pro
remark   geometric energy function parameters for distance geometry and
remark   simulated annealing.

set message off echo off end

! The values of the force constants are somewhat arbitrary. The aim
! is to make ALL of them stiff compared to the weight on the NOE
! term. The force constant for the angles is adjusted such that the
! 1-3 distance is approximately as well maintained as the 1-2 distance.
!
! All angles around tetrahedral carbons (type CT) have been set
! to the ideal methane value, 109.5 degrees, by JK.
!
! the non-bonded parameters have been modified such that they
! give approximately the large DISMAN radii with repel=0.9,
! and the small DISMAN radii (or the DISGEO radii) with
! repel= 0.75.

! for floating assignment, set KMENE to 0

!
remark corrected proline angles to Engh & Huber, Acta Cryst., A47, 392
(1991) values.
remark Needed to define a new atom type, CP, which is equivalent to their
remark CH2P atom type. JJK 9/22/95
!

                                                {* set energy constants *}
evaluate ($kbon = 1000)  ! kcal / mol-A^2
evaluate ($kang =  500)  ! kcal / mol-rad^2
evaluate ($kchi =  500)  ! kcal / mol-rad^2
evaluate ($kback = 500)
evaluate ($kmene =   0)   ! changed HS
evaluate ($kmtyl = 500)
evaluate ($kssbon = 1000)
evaluate ($kssang = 500)
evaluate ($kpla =  500)  ! kcal / mol-rad^2
evaluate ($kdih =    0)  ! kcal / mol-rad^2


! BONDS

 bonds     H    NA                $kbon     0.98
 bond      H    NH2               $kbon     0.98
 bond      H    NH1               $kbon     0.98
 bond      H    OH                $kbon     0.96
 bond      H    S                 $kbon     0.96
 bond      HA   CT                $kbon     1.08
 bond      HA   C                 $kbon     1.08
```

```
 bond      HC   NC2                $kbon     1.00
 bond      HC   NH1                $kbon     0.98
 bond      HC   NH3                $kbon     1.04
 bond      C    C                  $kbon     1.38
 bond      C    CT                 $kbon     1.53
 bond      C    N                  $kbon     1.341
 bond      C    NP                 $kbon     1.305
 bond      C    NR                 $kbon     1.305
 bond      C    NH1                $kbon     1.305
 bond      C    NH2                $kbon     1.305
 bond      C    NC2                $kbon     1.305
 bond      C    O                  $kbon     1.215
 bond      C    OC                 $kbon     1.22
 bond      C    OH                 $kbon     1.38
 bond      C    CA                 $kbon     1.400
 bond      CA   CA                 $kbon     1.400
 bond      CA   CB                 $kbon     1.404
 bond      CA   CN                 $kbon     1.400
 bond      CA   CT                 $kbon     1.510
 bond      CA   HA                 $kbon     1.080
 bond      CB   CN                 $kbon     1.419
 bond      CC   CT                 $kbon     1.504
 bond      CC   CV                 $kbon     1.375
 bond      CC   NA                 $kbon     1.385
 bond      CN   NA                 $kbon     1.380
 bond      CR   HA                 $kbon     1.080
 bond      CR   NA                 $kbon     1.343
 bond      CR   NB                 $kbon     1.3350
 bond      CT   CT                 $kbon     1.53
 bond      CT   N                  $kbon     1.466
 bond      CT   NH1                $kbon     1.49
 bond      CT   NH2                $kbon     1.49
 bond      CT   NH3                $kbon     1.49
 bond      CT   NC2                $kbon     1.49
 bond      CT   OH                 $kbon     1.42
 bond      CT   S                  $kbon     1.81
 bond      CV   HA                 $kbon     1.080
 bond      CV   NB                 $kbon     1.394
 bond      CX   CB                 $kbon     1.459
 bond      CX   CT                 $kbon     1.495
 bond      CX   CW                 $kbon     1.352
 bond      CW   HA                 $kbon     1.080
 bond      CW   NA                 $kbon     1.381
 bond      CP   CP                 $kbon     1.503 ! Unlike Engh & Huber,
JJK has 1.53 here for some reason. PN 12/8/2002
 bond      CP   CT                 $kbon     1.492
 bond      CP   N                  $kbon     1.473
 bond      CP   NH3                $kbon     1.473
 bond      CP   HA                 $kbon     1.08
 bond      S    S                  $kssbon   2.02
 bond      H    NB                 $kbon     0.98
 bond      CC   NB                 $kbon     1.385
 bond      CV   NA                 $kbon     1.394

! ANGLES

 angle     H    NH1  H             $kang     107.5
 angle     H    NH1  C             $kang     120.0
 angle     H    NH1  CT            $kang     120.0
 angle     H    NH2  H             $kang     120.0
 angle     H    NH2  C             $kang     120.0
```

```
 angle     H    NH2  CT            $kang     120.0
 angle     H    OH   CT            $kang     108.0
 angle     H    S    CT            $kang     108.0
 angle     H    OH   C             $kang     108.0
 angle     HC   NH3  HC            $kang     109.5
 angle     HC   NH3  CT            $kang     109.5
 angle     HC   NH3  CP            $kang     109.0 ! Modified to match Engh
& Huber angles for heavy atoms. PN 12/8/2002
 angle     HC   NC2  HC            $kang     120.0
 angle     HC   NC2  C             $kang     120.0
 angle     HC   NC2  CT            $kang     107.5
 angle     HA   C    C             $kang     120.0
 angle     HA   C    NH1           $kang     120.0
 angle     HA   C    NH2           $kang     120.0
 angle     HA   C    NR            $kang     120.0
 angle     HA   C    O             $kang     120.0
 angle     HA   CR   NA            $kang     124.2     !corrected by JK
 angle     HA   CR   NB            $kang     124.2     !corrected by JK
 angle     HA   CT   HA            $kang     109.5
 angle     HA   CT   C             $kang     109.5
 angle     HA   CT   CT            $kang     109.5
 angle     HA   CT   N             $kang     112.0 ! Modified to match Engh
& Huber angles for heavy atoms. PN 12/8/2002
 angle     HA   CT   NH1           $kang     109.5
 angle     HA   CT   NH3           $kang     109.5
 angle     HA   CT   NC2           $kang     109.5
 angle     HA   CT   OH            $kang     109.5 !corrected by JK
 angle     HA   CT   S             $kang     109.5
 angle     HA   CV   NB            $kang     125.05    !corrected by JK
 angle     HA   CW   NA            $kang     125.65    !corrected JK
 angle     C    C    C             $kang     126.5
 angle     C    C    CT            $kang     122.3
 angle     C    C    NH1           $kang     108.6
 angle     C    C    NP            $kang     109.5
 angle     C    C    NR            $kang     109.5
 angle     C    C    OH            $kang     122.3
 angle     C    CA   CA            $kang     120.000
 angle     C    CA   HA            $kang     120.0
 angle     C    CT   CT            $kang     109.5
 angle     C    CT   N             $kang     111.8
 angle     C    CT   NH1           $kang     109.5
 angle     C    CT   NH2           $kang     109.5
 angle     C    CT   NH3           $kang     109.5
 angle     C    N    CT            $kang     122.6
 angle     C    NH1  C             $kang     119.1
 angle     C    NH1  CT            $kang     120.0  !corrected by JK unq.
ARG
 angle     C    NC2  CT            $kang     107.5
 angle     C    NP   C             $kang     106.0
 angle     C    NR   C             $kang     106.0
 angle     CA   C    CA            $kang     120.0
 angle     CA   C    OH            $kang     120.0
 angle     CA   CA   CA            $kang     120.0
 angle     CA   CA   CB            $kang     120.0
 angle     CA   CA   CN            $kang     120.0
 angle     CA   CA   CT            $kang     120.0
 angle     CA   CA   HA            $kang     120.000
 angle     CA   CB   CN            $kang     118.0
 angle     CA   CN   CB            $kang     122.0
 angle     CA   CT   CT            $kang     109.5
 angle     CA   CT   HA            $kang     109.5000
```

```
 angle     CB   CA   HA            $kang     120.0
 angle     CB   CX   CT            $kang     128.6
 angle     CB   CX   CW            $kang     106.4
 angle     CB   CN   NA            $kang     104.40
 angle     CC   CT   CT            $kang     109.5
 angle     CC   CT   HA            $kang     109.5000
 angle     CC   CV   HA            $kang     125.05    !corrected by JK
 angle     CC   CV   NB            $kang     109.9000
 angle     CC   NA   CR            $kang     107.3000
 angle     CC   NA   H             $kang     126.300
 angle     CN   CA   HA            $kang     120.00
 angle     CN   NA   CW            $kang     111.6000
 angle     CN   NA   H             $kang     123.100
 angle     CR   NA   H             $kang     126.3000
 angle     CR   NB   CV            $kang     105.3000
 angle     CT   C    N             $kang     116.9
 angle     CT   C    NH1           $kang     117.5
 angle     CT   C    NH2           $kang     120.0
 angle     CT   C    O             $kang     121.25  !corrected by JK (pept
planarity)
 angle     CT   C    OH            $kang     117.5
 angle     CT   C    OC            $kang     118.0
 angle     CT   CC   CV            $kang     131.900
 angle     CT   CC   NA            $kang     122.2000
 angle     CT   CT   CT            $kang     109.5 !JK
 angle     CT   CT   N             $kang     103.0
 angle     CT   CT   NH1           $kang     109.5
 angle     CT   CT   NH2           $kang     109.5
 angle     CT   CT   NH3           $kang     109.5
 angle     CT   CT   NC2           $kang     109.5
 angle     CT   CT   OH            $kang     109.5 !corrected by JK
 angle     CT   CT   S             $kang     109.5
 angle     CT   CX   CW            $kang     125.0000
 angle     CT   N    CT            $kang     119.0
 angle     CT   S    CT            $kang     97.20
 angle     CT   S    S             $kssang   104.2
 angle     CV   CC   NA            $kang     105.900
 angle     CW   NA   H             $kang     125.300
 angle     CX   CB   CN            $kang     108.800
 angle     CX   CT   CT            $kang     109.5
 angle     CX   CT   HA            $kang     109.5
 angle     CX   CW   HA            $kang     125.65   !corrected by JK
 angle     CX   CW   NA            $kang     108.7

 angle     CT   CT   CP            $kang     104.500 !\
 angle     CT   CP   CP            $kang     106.100 ! \
 angle     CP   CP   N             $kang     103.200 !  > from parhcsdx.pro
 angle     C    N    CP            $kang     125.000 ! /
 angle     CT   N    CP            $kang     112.000 !/
 angle     CP   CP   NH3           $kang     103.200
 angle     C    NH3  CP            $kang     125.000
 angle     CT   NH3  CP            $kang     112.000
 angle     HA   CP   HA            $kang     109.5
 angle     HA   CP   CP            $kang     110.5 ! Modified to match Engh
& Huber angles for heavy atoms. PN 12/8/2002
 angle     HA   CP   CT            $kang     109.5
 angle     HA   CT   CP            $kang     111.5 ! Modified to match Engh
& Huber angles for heavy atoms. PN 12/8/2002
 angle     HA   CP   N             $kang     111.5 ! Modified to match Engh
& Huber angles for heavy atoms. PN 12/8/2002
 angle     HA   CP   NH3           $kang     111.5 ! Modified to match Engh
```

```
& Huber angles for heavy atoms. PN 12/8/2002

 angle     N    C    O             $kang     122.0
 angle     NA   CR   NB            $kang     111.60
 angle     NH1  C    NC2           $kang     120.0  !corrected by JK
 angle     NH1  C    NR            $kang     117.0
 angle     NH1  C    O             $kang     121.25 !corrected by JK (pept
planarity)
 angle     NH2  C    O             $kang     120.6
 angle     NC2  C    NC2           $kang     120.0  !corrected by JK
 angle     O    C    OH            $kang     124.5
 angle     OC   C    OC            $kang     124.0  !corrected by JK
 angle     CA   CN   NA            $kang     133.6  !trp addition
 angle     CA   CB   CX            $kang     133.2  !trp addition

 angle     H    NB   CV            $kang     120.0
 angle     H    NB   CR            $kang     120.0

! IMPROPERS

! For dihedrals and impropers, the following convention was adopted:
! All dihedral terms maintaining planarity (esp. omega) have been
! converted into impropers. The only dihedrals left are around
! rotatable bonds.

 improper  H    X    X    C        $kpla    0    0.0
 improper  H    X    X    NH1      $kpla    0    0.0
 improper  H    X    X    NH2      $kpla    0    0.0
 improper  H    X    X    O        $kpla    0    0.0
 improper  HC   X    X    NH1      $kpla    0    0.0
 improper  HC   X    X    NC2      $kpla    0    0.0
 improper  HC   X    X    NH3      $kpla    0    0.0
 improper  HA   X    X    C        $kpla    0    0.0
 improper  C    X    X    C        $kpla    0    0.0
 improper  C    X    X    CT       $kpla    0    0.0
 improper  C    X    X    N        $kpla    0    0.0
 improper  C    X    X    NH1      $kpla    0    0.0
 improper  C    X    X    NH2      $kpla    0    0.0
 improper  C    X    X    NC2      $kpla    0    0.0
 improper  C    X    X    NR       $kpla    0    0.0
 improper  C    X    X    O        $kpla    0    0.0
 improper  C    X    X    OH       $kpla    0    0.0
 improper  C    X    X    OC       $kpla    0    0.0
 improper  CT   X    X    N        $kpla    0    0.0
 improper  CT   X    X    NH1      $kpla    0    0.0
 improper  CT   X    X    NH3      $kpla    0    0.0
 improper  CT   X    X    NC2      $kpla    0    0.0
 improper  CT   X    X    NR       $kpla    0    0.0
 improper  NH1  X    X    NH1      $kpla    0    0.0
 improper  NH1  X    X    NR       $kpla    0    0.0
 improper  NH1  CT   NC2  HC       $kpla    0    0.0    ! Arg
 improper  CT   C    NH2  H        $kpla    0    0.0    ! Asn and Gln

! note the way the omega planarity is defined which allows switch
! between trans and cis by a patch.

 improper  CT   C    NH1  CT       $kback   0  180.0    ! new trans peptide
bond
 improper  CT   C    N    CT       $kback   0  180.0    ! proline
 improper  CP   C    N    CT       $kback   0  180.0    ! proline
 improper  O    C    NH1  CT       $kback   0    0.0    ! CO planarity
```

```
 improper  O    C    N    CT       $kback   0    0.0    ! CO planarity,
proline
 improper  H    NH1  C    CT       $kback   0    0.0    ! NH peptide
planarity
 improper  C    CT   CT   NH1      $kback   0  180.0    ! trans peptide
bond
 improper  C    CT   NH1  CT       $kback   0  180.0    ! cis   peptide
bond
 improper  C    CT   CT   N        $kback   0  180.0    ! Pro trans peptide
bond
 improper  C    CT   N    CT       $kback   0  180.0    ! Pro cis   peptide
bond
 improper  C    O    NH1  CT       $kback   0    0.0    !! new cis CO
planarity
 improper  C    O    N    CT       $kback   0    0.0    !! new cis CO
planarity, proline
 improper  NH1  H    C    CT       $kback   0    0.0    !! new cis NH
peptide planarity
 improper  N    CT   CT   CP       $kback   0   25.     ! proline ring
pucker
 improper  NH3  CT   CT   CP       $kback   0   25.     ! proline ring
pucker
 improper  C    CP   N    CT       $kback   0  180.0    ! Pro cis peptide
5/21/96

! 65.977 degrees for the chirality restraints are from
! isolated CAs minimized with bonds and angles only --JK

 improper  HA   NH1  C    CT       $kchi    0   65.977  ! CA chirality
 improper  HA   N    C    CT       $kchi    0   65.977  ! Pro CA chirality
 improper  HA   NH3  C    CT       $kchi    0   65.977  ! N-terminal CA
chirality
 improper  HA   C    NH1  CT       $kchi    0   65.977  ! D  CA chirality
 improper  HA   C    N    CT       $kchi    0   65.977  ! D  Pro CA
chirality
 improper  HA   C    NH3  CT       $kchi    0   65.977  ! D  N-terminal CA
chirality
 improper  HA   CT   OH   CT       $kchi    0   65.977  ! Thr CB chirality
 improper  HA   CT   CT   CT       $kmene   0   -65.977  ! val,
leu,chirality
 improper  CT   HA   CT   CT       $kchi    0   76.0     ! ile chirality -
by HS

! hold tetrahedral groups in the proper positions
! these were also computed by minimising isolated groups

 improper  HA   HA   CT   HA       $kmtyl   0   -66.514  ! methyl
 improper  HA   HA   S    HA       $kmtyl   0   -66.0    ! met methyl
 improper  HC   HC   CT   HC       $kmtyl   0   -66.0    ! amine for lys &
N terminus
 improper  HC   HC   CT   CP       $kmtyl   0   -70.784  ! CP, N-terminal
pro
 improper  HA   HA   CT   CT       $kmene   0   -70.874  ! methylene
 improper  HA   HA   CT   CA       $kmene   0   -70.874  ! methylene phe
 improper  HA   HA   CT   CX       $kmene   0   -70.874  ! methylene trp
 improper  HA   HA   CT   CC       $kmene   0   -70.874  ! methylene his
 improper  HA   HA   CT   C        $kmene   0   -70.874  ! methylene glu,
asp
 improper  HA   HA   CT   CP       $kmene   0   -70.874  ! methylene pro
 improper  HA   HA   CP   N        $kmene   0   -70.874  ! methylene pro
 improper  HA   HA   CP   NH3      $kmene   0   -70.874  ! methylene pro
```

```
 improper  HA   HA   NH1  C        $kmene   0   -70.874  ! methylene gly
 improper  HA   HA   NH3  C        $kmene   0   -70.874  ! stereo GLY CA at
NTER (P. Driscoll 7/25/93)
 improper  HA   HA   CT   NH1      $kmene   0   -70.874  ! methylene arg
 improper  HA   HA   CT   NH3      $kmene   0   -70.874  ! methylene lys
 improper  HA   HA   CT   S        $kmene   0   -73.230  ! methylene cys,
met
 improper  HA   HA   CT   OH       $kmene   0   -71.884  ! methylene ser
 improper  HA   HA   CT   N        $kmene   0   -70.874  ! methylene arg

! hold rings flat (from parallhgeo)
! trp
 improper   CB   CN   CA   CA      $kpla    0    0.0
 improper   CN   CA   CA   CA      $kpla    0    0.0
 improper   CA   CA   CA   CA      $kpla    0    0.0
 improper   CA   CA   CA   CB      $kpla    0    0.0
 improper   CA   CA   CB   CN      $kpla    0    0.0
 improper   CA   CB   CN   CA      $kpla    0    0.0
 improper   CW   NA   CN   CA      $kpla    0  180.0
 improper   CW   CX   CB   CA      $kpla    0  180.0
 improper   NA   CN   CA   CA      $kpla    0  180.0
 improper   NA   CN   CB   CA      $kpla    0  180.0
 improper   CX   CB   CA   CA      $kpla    0  180.0
 improper   CX   CB   CN   CA      $kpla    0  180.0
 improper   HA   CA   CA   CA      $kpla    0  180.0
 improper   H    NA   CN   CB      $kpla    0  180.0
 improper   HA   CW   NA   CN      $kpla    0  180.0
 improper   CT   CX   CB   CN      $kpla    0  180.0
!phe
 improper   CT   CA   CA   CA      $kpla    0  180.0
!tyr
 improper   OH   C    CA   CA      $kpla    0  180.0
 improper   HA   CA   CA   C       $kpla    0  180.0
 improper   HA   CA   C    CA      $kpla    0  180.0

! improper   CA   C    CA   HA      $kpla    0    0.0
 improper   CA   CA   C    CA      $kpla    0    0.0
 improper   CA   CA   C    HA      $kpla    0    0.0
 improper   CA   CA   CA   C       $kpla    0    0.0
 improper   CA   CA   CB   HA      $kpla    0    0.0
 improper   CA   CA   CN   CA      $kpla    0    0.0
 improper   CA   CB   CA   CA      $kpla    0    0.0
 improper   CA   CN   CA   HA      $kpla    0    0.0
 improper   CB   CX   CN   CA      $kpla    0    0.0
 improper   CC   CT   NA   CV      $kpla    0    0.0
 improper   CC   NA   CR   NB      $kpla    0    0.0
 improper   CN   CB   CA   NA      $kpla    0    0.0
 improper   CN   CB   CX   CW      $kpla    0    0.0
 improper   CN   NA   CW   CX      $kpla    0    0.0
 improper   CR   NA   NB   HA      $kpla    0    0.0
 improper   CR   NB   CV   CC      $kpla    0    0.0
 improper   CV   CC   NA   CR      $kpla    0    0.0
 improper   CV   NB   CC   HA      $kpla    0    0.0
 improper   CW   CX   NA   HA      $kpla    0    0.0
 improper   CW   NA   CN   CB      $kpla    0    0.0
 improper   CX   CW   CB   CT      $kpla    0    0.0
 improper   NA   CN   CB   CX      $kpla    0    0.0
 improper   NA   CR   CC   H       $kpla    0    0.0
 improper   NA   CR   NB   CV      $kpla    0    0.0
 improper   NA   CW   CN   H       $kpla    0    0.0
```

```
 improper   NA   CW   CX   CB       $kpla    0    0.0
 improper   NB   CV   CC   NA       $kpla    0    0.0

 improper   NB   CR   CV   H        $kpla    0    0.0


! DIHEDRALS

 dihedral  CA   CA   CT   CT       $kdih    3    0.0
 dihedral  CW   CX   CT   CT       $kdih    3    0.0
 dihedral  NA   CC   CT   CT       $kdih    3    0.0
 dihedral  X    NH1  CT   X        $kdih    3    0.0  ! chi1 - chi4
 dihedral  X    CT   CT   X        $kdih    3    0.0  ! chi1 - chi4
 dihedral  X    C    CT   X        $kdih    3    0.0  ! chi1 - chi4
 dihedral  X    S    CT   X        $kdih    3    0.0  ! chi1 - chi4

! the non-bonded parameters are approximately the same as
! DISMAN's large radii for repel=0.9, and as DISMAN's small
! radii for repel=0.75. (ECEPP2)
! the epsilon values are generally not used (and should not be)
! with this force field
! the radius is sigma*2^(-5/6)
!
!                   eps     sigma       eps(1:4) sigma(1:4)  repel:  1.0
0.9     0.8     0.75
!
radii
 nonbonded  C       0.0903   3.3409      0.0903   3.3409   !         1.875
1.688   1.5     1.406
 NONBonded  CA      0.120    3.3409      0.120    3.3409
 NONBonded  CB      0.145    3.3409      0.145    3.3409
 NONBonded  CC      0.145    3.3409      0.145    3.3409
 NONBonded  CN      0.145    3.3409      0.145    3.3409
 NONBonded  CP      0.1450   3.3409      0.1450   3.3409
 NONBonded  CR      0.1200   3.3409      0.1200   3.3409
 nonbonded  CT      0.0903   3.3409      0.0903   3.3409
 NONBonded  CV      0.1200   3.3409      0.1200   3.3409
 NONBonded  CW      0.1200   3.3409      0.1200   3.3409
 NONBonded  CX      0.1450   3.3409      0.1450   3.3409
 nonbonded  H       0.0498   2.2272      0.0498   2.2272   !         1.250
1.125   1.0     0.9375
 nonbonded  HA      0.0045   2.2272      0.0045   2.2272
 nonbonded  HC      0.0498   2.2272      0.0498   2.2272
 nonbonded  N       0.1592   3.0068      0.1592   3.0068   !         1.688
1.519   1.350   1.266
 NONBonded  NA      0.1592   3.0068      0.1592   3.0068
 NONBonded  NB      0.1592   3.0068      0.1592   3.0068
 nonbonded  NC2     0.1592   3.0068      0.1592   3.0068
 nonbonded  NH1     0.1592   3.0068      0.1592   3.0068
 nonbonded  NH2     0.1592   3.0068      0.1592   3.0068
 nonbonded  NH3     0.1592   3.0068      0.1592   3.0068
 nonbonded  O       0.2342   2.7755      0.2342   2.7755   !         1.558
1.402   1.246   1.168
 nonbonded  OC      1.0244   2.7755      1.0244   2.7755
 nonbonded  OH      0.2342   2.7755      0.2342   2.7755
 nonbonded  S       0.0239   3.7458      0.0239   3.7458   !         2.102
1.892   1.682   1.577

! the following nbfixes allow hydrogen bonding
! the distance used is (2A/B)^(1/6)*repel
distances
```

```
!                            A    B   A1-4  B1-4
 nbfix      H      NB     44.2  1.0  44.2  1.0              !         2.111
1.900   1.689   1.583
 nbfix      H      O      44.2  1.0  44.2  1.0
 nbfix      H      OC     44.2  1.0  44.2  1.0
 nbfix      H      OH     44.2  1.0  44.2  1.0
 nbfix      HC     NB     44.2  1.0  44.2  1.0
 nbfix      HC     O      44.2  1.0  44.2  1.0
 nbfix      HC     OC     44.2  1.0  44.2  1.0
 nbfix      HC     OH     44.2  1.0  44.2  1.0

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